LONG-TIME BEHAVIOUR OF TIME-DEPENDENT DENSITY FUNCTIONAL THEORY

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Abstract. The density functional theory (DFT) is a remarkably successful theory of electronic structure of matter. At the foundation of this theory lies the Kohn-Sham (KS) equation. In this paper, we describe the long-time behaviour of the time-dependent KS equation. Assuming weak self-interactions, we prove global existence and scattering in (almost) the full "short-range" regime. This is achieved with new and simple techniques, naturally compatible with the structure of the DFT and involving commutator vector fields and non-abelian versions of Sobolev-Klainerman-type spaces and inequalities.

Contents

1. Introduction

1.1. **The DFT equation.** The density functional theory (DFT) is a remarkably successful theory of electronic structure of matter (see e.g. [17, 19, 20, 27] for some reviews). It naturally applies not just to electrons, but to any fermion gas, say, of atoms, molecules or nucleons considered as point particles.

At the foundation of the DFT is the seminal Kohn-Sham equation (KSE). Originally written in the stationary context and for pure states (represented through the Slater determinant by orthonormal systems of n functions, called orbitals), the KSE has a natural extension to the time-dependent framework (see e.g. [2, 4, 5, 10, 13, 34]). Moreover, it can be rewritten in terms of orthogonal projections and then extended to density operators, i.e. positive, trace-class operators (see for example [23, 8, 10] and references therein) and takes the following form:

$$\frac{\partial \gamma}{\partial t} = i[h_\gamma, \gamma], \qquad h_\gamma := -\Delta + f(\gamma), \tag{1.1}$$

with $\gamma = \gamma(t)$ a *positive* operator-family on $L^2(\mathbb{R}^d)$ and f mapping a class of self-adjoint operators on $L^2(\mathbb{R}^d)$ into itself. In addition, we require that f depends on γ through the function

$$\rho_\gamma(x,t) := \gamma(x,x,t),$$

where $\gamma(x,y,t)$ are integral kernels of $\gamma(t)$, i.e. there is $g : L^1_{\mathrm{loc}}(\mathbb{R}^d,\mathbb{R}) \to L^2_{\mathrm{loc}}(\mathbb{R}^d,\mathbb{R})$, such that

$$f(\gamma) = g(\rho_\gamma),$$

where $g(\rho)$ on the right-hand side is considered as a multiplication operator. $L^2(\mathbb{R}^d)$ is called the one-particle space, $\gamma(t)$, the *density operator* at time t and ρ_γ, the *one-particle charge density.*

Initial conditions are taken to be non-negative operators, $\gamma|_{t=0} = \gamma_0 \geq 0$ and, for fermions, in addition, satisfying $\gamma_0 \leq 1$, which encodes the Pauli exclusion principle. It is easy to show that, under suitable conditions on g, the solutions have the same properties, $0 \leq \gamma$ (≤ 1). (In fact, all eigenvalues of γ are conserved under the evolution.)

Since $\gamma \geq 0$, we have that $\rho_\gamma(x,t) := \gamma(x,x,t) \geq 0$ and, since it is interpreted as the one-particle (charge) density, $\mathrm{Tr}\gamma = \int \rho_\gamma dx$ is the total number of particles.

Since h_γ depends on γ only through the density ρ_γ, $h_\gamma \equiv h(\rho_\gamma)$, Eq. (1.1) is equivalent to the equation for the density ρ,

$$\frac{\partial \rho}{\partial t} = \mathrm{den}(i[h(\rho),\gamma]),$$

where $\mathrm{den}(A) \equiv \rho_A$, the density for an operator A. Hence is the term *density functional theory* (DFT).

We assume that the nonlinearity or self-interaction $f(\gamma)$ is *translation, rotation and gauge covariant* in the sense that

$$U_\lambda f(\gamma) U_\lambda^{-1} = f(U_\lambda \gamma U_\lambda^{-1}), \tag{1.2}$$

where U_λ is either the translation, rotation and gauge transformation, respectively given by

$$\begin{aligned} U_\lambda^{\mathrm{tr}} &: f(x) \mapsto f(x+\lambda), \qquad \lambda \in \mathbb{R}^d, \\ U_\lambda^{\mathrm{rot}} &: f(x) \mapsto f(\lambda^{-1}x), \qquad \lambda \in O(d), \\ U_\lambda^{\mathrm{g}} &: f(x) \mapsto e^{i\lambda} f(x), \qquad \lambda \in \mathbb{R}. \end{aligned}$$

For $f(\gamma) = g(\rho_\gamma)$, (1.2) and $U_\lambda \rho_\gamma = \mathrm{den}(U_\lambda \gamma U_\lambda^{-1})$ imply that $g(\rho_\gamma)$ satisfies

$$U_\lambda g(\rho) U_\lambda^{-1} = g(U_\lambda \rho). \tag{1.3}$$

Here $g(\rho)$ is considered as a multiplication operator, and ρ as a function.

A standard example of self-interaction in physics is the sum of a *Hartree-type* nonlinearity and a local *exchange-correlation term* of the form

$$g(\rho) = v * \rho + \mathrm{xc}(\rho) \tag{1.4}$$

for some potential $v = v(x)$ and some function $\mathrm{xc} = \mathrm{xc}(\rho)$. Important cases of v in (1.4) are $v(x) = \lambda/|x|$ (the Coulomb or Newton potential, if $d = 3$) and $v(x) = \lambda\delta(x)$ (the local potential, which can also considered as part of the exchange term). An important example of exchange-correlation term is the Dirac one, $\mathrm{xc}(\rho) = -c\rho^{1/3}$, $c > 0$, in 3 dimensions.

In Subsection 1.2 we will define a general class of self-interactions that we are going to consider.

In general, one would like to address the following problems

- Global existence vs blowup;
- Asymptotic behaviour as $t \to \infty/T_{\text{blowup}}$ (scattering theory, return to equilibrium vs. blowup dynamics);
- Static, self-similar and travelling wave solutions and their stability;
- Macroscopic limit (effective equations).

The existence theory for the standard Hartree and Hartree-Fock equations (which are similar and closely related to (1.1)) with trace class initial data, $\mathrm{Tr}\gamma_0 < \infty$, was developed in [3, 6, 7].

For the Hartree equation Lewin and Sabin [23, 24] studied the harder case of non-trace class solutions. For initial conditions given by suitable trace-class perturbations of translation invariant states $\gamma_f = f(-\Delta)$, the authors established global well-posedness [23] in dimensions $d = 2, 3$ as well as dispersive properties of the solutions and scattering for $d = 2$ [24]. These results have been extended to the more singular case of local nonlinearities ($v(x) = \lambda\delta(x)$) by Chen, Hong and Pavlović, who proved global well-posedness in dimensions $d = 2, 3$ and zero temperature [8]. The same authors also proved scattering results in the case of dimension 3 and higher [9], left open in [24]. Finally, we mention the recent work of Collot and de Suzzoni [11] who proved analogues of the results of [24, 9] for the Hartree equation for a random variable in $d \geq 4$.

For classical papers on scattering theory for Schrödinger and Hartree type evolution equations we refer to Strauss [33] and Ginibre-Velo [12]. See also the works [15, 18] and references therein, on the scattering critical cases and the work on the Chern-Simons-Schrödinger equation by Oh and the first author [28], where weighted energy estimates are done covariantly, by adapting the standard Schrödinger "vector field" (see j_ℓ in (1.12)) to the covariant structure of the equations. See also [30, 31] on the use of related ideas in the context of quantum scattering theory.

1.2. **Results.** For $p \in [1, \infty]$, we let $L^p(\mathbb{R}^d)$ be the standard Lebesgue spaces on $\mathbb{R}^d$ with the norms denoted by $\|\cdot\|_{L^p}$ or $\|\cdot\|_p$. We also let L^r_w denote the weak L^r space. We assume that $f(\gamma)$ is of the form

$$f(\gamma) = g(\rho) = \lambda_1 v * \rho + \lambda_2 \rho^\beta, \tag{1.5}$$

with

$$v \in L^r_w(\mathbb{R}^d), \quad r \in (1, d), \qquad \text{and} \qquad \beta > 1/\min(d, 2). \tag{1.6}$$

Note that the convolution term is omitted for $d = 1$.

To keep the exposition simple we let $d \leq 3$, and will make a few comments about extensions to the higher dimensional cases in Remarks 1.3 and 7.2 below.

Let I^r denote the space of bounded operators satisfying

$$\|A\|_{I^r} := (\mathrm{Tr}(A^*A)^{r/2})^{1/r} < \infty, \tag{1.7}$$

a trace ideal or non-commutative L^r−space.

We say that Eq (1.1) is *asymptotically complete*, or has the *short-range scattering property*, if and only if, for any initial condition $\gamma_0 \in I^1$, there is an operator $\gamma_\infty \in I^1$ independent of t, such that the solution $\gamma(t)$ to equation (1.1) satisfies, as $t \to \infty$,

$$\left\|\gamma(t) - e^{it\Delta}\gamma_\infty e^{-i\Delta t}\right\|_{I^1} \to 0. \tag{1.8}$$

Our main result is

Theorem 1.1. *Consider* (1.1) *with* $g(\rho)$, *satisfying* (1.5)-(1.6), *and initial datum* $\gamma_0 = \gamma_0^* = \gamma(t=0)$ *satisfying*

$$\|\langle x\rangle^b \gamma_0 \langle x\rangle^b\|_{I^1} + \|\langle\nabla\rangle^b \gamma_0 \langle\nabla\rangle^b\|_{I^1} < \infty, \tag{1.9}$$

for some integer $b > d/2$. *Then, for* $|\lambda_1|, |\lambda_2|$ *sufficiently small depending on* $\|\langle x\rangle^b \gamma_0 \langle x\rangle^b\|_{I^1}$, *the equation* (1.1) *with the initial datum* γ_0

(i) *is globally well-posed;*
(ii) *is asymptotically complete (see* (1.8)*).*

Theorem 1.1 follows from Theorem 3.3 and Proposition 3.2 formulated in Section 3 below. Statement (i) in Theorem 1.1 is not new, and can be obtained under milder assumptions on the data. The main new result is the scattering property, (ii). Importantly, our results are given in the natural (weighted) trace norms.

The class of self-interactions that we actually treat is larger than (1.5)–(1.6), see Remark 1.2 below.

For convolution potentials that have stronger integrability properties and no exchange terms, scattering results also follow from the cited works [24, 8, 9]. Here we are able to cover the full subcritical range for the convolution part, and the almost full subcritical range for the xc term. As a byproduct of our proof, we obtain that the solutions given in Theorem 1.1 also enjoy the local decay estimate (3.21).

In view of our analysis it is natural to formulate the following conjectures.

Conjecture 1 (Exponent β)**.** *The range of exponents* β *in* (1.6) *for which short-range scattering holds is*

$$\beta > 1/d.$$

In this respect our result is sharp in dimensions 1 and 2, see (1.5), while it is not optimal for $d = 3$ (and $d > 3$, see Remark 1.3).

Conjecture 2 (Scattering critical case)**.** *For* (1.5) *with* $v = |x|^{-\alpha}$,

$$g(\rho) = \lambda_1|x|^{-\alpha} * \rho + \lambda_2\rho^\beta \quad \text{with} \quad 0 < \alpha \leq 1, \quad 0 < \beta \leq 1/d,$$

modified scattering holds. In particular, for $\alpha = 1$ *and* $\beta = 1/d$, *we expect that*

$$\left\|\gamma(t) - e^{-i(-t\Delta + g_\infty(-i\nabla)\,\log t)}\gamma_\infty e^{i(-t\Delta + g_\infty(-i\nabla)\,\log t)}\right\|_{I^1} \to 0,$$

as $t \to \infty$ (with some algebraic rate), where $\gamma_\infty \in I^1$ is time independent, and g_∞ is a time-independent operator which depends nonlinearly on γ_∞.

Unlike most of the previous research on the Hartree, Hartree-Fock and Kohn-Sham equations, which uses the formulation of the equations in terms of the eigenfunctions of γ, we deal with the operator γ directly. There are three basic ingredients in our approach:

(i) Passing to the Hilbert space I^2 of Hilbert-Schmidt operators with the inner product

$$\langle \kappa, \kappa' \rangle_{I^2} := \mathrm{Tr}(\kappa^* \kappa'). \tag{1.10}$$

by going from γ to, roughly speaking, $\kappa := \sqrt{\gamma}$;

(ii) Deriving almost conservation laws for non-abelian analogues of weighted Sobolev spaces

$$W^s := \{\kappa \in I^2 \, : \, \sum_{|\alpha| \le s} \|J^\alpha \kappa\|_{I^2} < \infty\}, \tag{1.11}$$

based on the space I^2 with the smoothness grading provided by operators

$$J_\ell \kappa := [j_\ell, \kappa], \qquad j_\ell := x_\ell - 2p_\ell t, \qquad p_\ell := -i\partial_\ell. \tag{1.12}$$

Here, as usual, $J^\alpha := \prod_i J_{\ell_i}^{\alpha_i}$ for $\alpha := (\alpha_i)$. Note that $W^0 = I^2$. Since J_ℓ is self-adjoint on (a dense subset of) I^2, one can define J_ℓ^r, for general non-integer r, by the operator calculus. In this paper, however, we will only use the spaces spaces W^s with integer s.

(iii) Using a new class of local norms for Hilbert-Schmidt operators, and establishing a non-commutative version of Gagliardo-Nirenberg-Klainerman-type estimates which yield bounds on these local norms of κ, and eventually imply the desired estimates on γ.

Remark 1.2 (Class of nonlinearities). We can treat a wider class of self-interactions than (1.5)-(1.6):

$$f(\gamma) = g(\rho_\gamma) = \lambda_1 g_1(\rho) + \lambda_2 g_2(\rho) \tag{1.13}$$

with $\lambda_1, \lambda_2 \in \mathbb{R}$ and the following assumptions on g_1 and g_2:

$$\|g_1(\rho)\|_\infty \lesssim \|\rho\|_q^a, \quad \text{for some} \quad a \ge 1 \quad \text{with} \quad a(1 - 1/q) > 1/d, \tag{1.14}$$

and its Gâteaux derivatives[1] satisfy

$$\|dg_1(\rho)\xi\|_p \lesssim \|\xi\|_q, \tag{1.15}$$

$$\|d^2 g_1(\rho)\xi\eta\|_p \lesssim \|\xi\|_{q'} \|\eta\|_{q'}, \tag{1.16}$$

[1]The k-th Gâteaux derivative could be defined by induction either as

$$d^k g_1(\rho)\xi_1\xi_2 \dots \xi_k := d(d^{k-1} g_1(\rho)\xi_1\xi_2 \dots \xi_{k-1})\xi_k,$$

or

$$d^k g_1(\rho)\xi_1\xi_2 \dots \xi_k := \prod_1^k \partial_{s_j}|_{s_i=0\forall i} g(\rho + \sum_1^k s_j \xi_j).$$

for some indexes (p, q, q') with[2]

$$p \geq d, \qquad q \leq \frac{d}{d-2}, \qquad 1 \leq q' \leq 2, \tag{1.17}$$

$$1 + 1/p - 1/q > 1/d, \qquad 2 + 1/p - 2/q' > 1/d; \tag{1.18}$$

and, for bounded ρ,

$$|g_2(\rho)| \lesssim \rho^\beta, \tag{1.19}$$

$$|d^k g_2(\rho)| \lesssim \rho^{\beta-k}, \qquad k = 1, 2, \tag{1.20}$$

where the power β satisfies (notice the difference with (1.6))

$$\begin{cases} \beta \geq 1/2, & d = 3 \\ \beta > 1/2, & d = 2 \\ \beta > 1, & d = 1. \end{cases} \tag{1.21}$$

Remark 1.3 (Higher dimensions). For $d \geq 4$, we have to add conditions on the higher (Gâteaux) derivatives of g. For example, the natural generalization of (1.15)-(1.16) with (1.18) would be the following assumption: there exist $(p, q, q_1, \dots, q_k)$ such that

$$\|d^k g_1(\rho)\xi_1\xi_2 \dots \xi_k\|_p \lesssim \prod_{i=1}^k \|\xi_i\|_{q_i}, \qquad k + 1/p - 1/q_1 \dots - 1/q_k > 1/d,$$

for all $k \leq [d/2] + 1$.

For g_2 one would instead assume (1.19) and (1.20) for all $k \leq [d/2] + 1$, As for the restriction analogous to (1.21), our current argument would require $\beta \geq (1/2)[d/2]$; see also Remark 7.2.

Remark 1.4 (Non-self-adjoint extension). We considered (1.1) on self-adjoint operators. By extending $f(\gamma)$ to non-self-adjoint operators, we can extend (1.1) to non-self-adjoint γ's. Then, assuming $f(\gamma^*) = f(\gamma)^*$ (or $g(\bar{\rho}) = \bar{g}(\rho)$) and extending condition (1.14) on g appropriately, we can show that

$$\alpha_t(\gamma^*) = \alpha_t(\gamma)^*, \tag{1.22}$$

where $\alpha_t(\gamma_0) := \gamma(t)$, the solution to (1.1) with the initial condition. $\gamma(t = 0) = \gamma_0$, and, in particular, $\gamma_0^* = \gamma_0 \Longrightarrow \gamma(t)^* = \gamma(t)$.

Remark 1.5. In the context of the Schrödinger evolution, the operators $j_t := x - 2pt$, $p := -i\nabla$, have been used in several works to obtain a priori estimates on solutions, see for example [15, 18, 30, 31].

[2] There is no restriction on q if $d = 1, 2$.

Remark 1.6. The operators $j_t := x - 2pt$ are the generators of the Galilean boost $U_{v,t}$: $\psi(x,t) \to e^{i(v\cdot x - |v|^2 t)}\psi(x - 2vt, t)$, which can be written as

$$U_{v,t} := e^{i(v\cdot x-|v|^2t)}e^{-2v\cdot\nabla t} = e^{iv\cdot(x-2pt)} = e^{iv\cdot j_t}. \tag{1.23}$$

(The second equality above follows from the Baker-Campbell-Hausdorff formula.) This is lifted to a space of operators as

$$\kappa \to U_{v,t}\kappa U_{v,t}^{-1} = e^{iv\cdot J_t}\kappa. \tag{1.24}$$

The paper is organized as follows. In Section 2 we recall several properties of (1.1) and give a definition of scattering criticality. In Section 3 we present our general strategy: we introduce a "half-density" κ, such that $\kappa^*\kappa = \gamma$ and derive an equation for it; we then state our main results concerning κ and show how these imply Theorem 1.1. Section 4 contains the proof of a non-abelian version of a Gagliardo-Nirenberg-Klainerman-type inequality, and Section 5 some simple estimates on densities. In Section 6 we estimate the evolution of the weighted energy, and then use this in Section 7 to prove the main a priori bounds for the weighted norms of κ, see (1.11). Finally, in Section 8 we prove a local existence result and continuity criterion for κ, and combine it with the a priori weighted bounds to complete the proof of global well-posedness and scattering.

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2. Properties of KSE

Symmetries and conserved quantities. The equation (1.1) is invariant under the *translation* and *rotation* transformations,

$$T_h^{\text{trans}} : \gamma \mapsto U_h\gamma U_h^{-1} \quad \text{and} \quad T_\rho^{\text{rot}} : \gamma \mapsto U_\rho\gamma U_\rho^{-1}, \tag{2.1}$$

for any $h \in \mathbb{R}^d$ and any $\rho \in O(d)$. Here U_h and U_ρ are the standard translation and rotation transforms $U_h : \phi(x) \mapsto \phi(x+h)$ and $U_\rho : \phi(x) \mapsto \phi(\rho^{-1}x)$.

Note that (1.1) has no gauge symmetry, unless it is coupled to the Maxwell equations.

The conserved energy and the number of particles are given by

$$E(\gamma) := \mathrm{Tr}(h\gamma) + G(\rho_\gamma), \tag{2.2}$$

$$N(\gamma) := \mathrm{Tr}\gamma = \int \rho_\gamma, \tag{2.3}$$

where $h := -\Delta$ and, recall, $\rho_\gamma(x) := \gamma(x,x)$ and $G(\rho)$ is an anti-L^2-gradient of $g(\rho)$, i.e. $d_\gamma G(\rho_\gamma)\xi = \mathrm{Tr}(g(\rho_\gamma)\xi)$. $G(\rho)$ is the energy due to direct electrostatic self-interaction of the charge distribution ρ_γ and the exchange-correlation energy, see (1.4). If $g(\rho) = v * \rho + \lambda\rho^\beta$, then

$$G(\rho_\gamma) = \frac{1}{2}\mathrm{Tr}((v*\rho_\gamma)\gamma) + \frac{\lambda}{\beta+1}\int \rho^{\beta+1} = \frac{1}{2}\int \rho_\gamma v * \rho_\gamma dx + \frac{\lambda}{\beta+1}\int \rho^{\beta+1}.$$

Hamiltonian structure. (1.1) is a Hamiltonian system with the Hamiltonian given by the energy (2.2) and the Poisson bracket generated by the operator $J = J(\gamma) : A \to i[A, \gamma]$ so that (1.1) can be rewritten as

$$\frac{\partial \gamma}{\partial t} = J(\gamma)\nabla E(\gamma) \tag{2.4}$$

where $\nabla E(\gamma)$ is defined by $dE(\gamma)\xi = \mathrm{Tr}(\xi \nabla E(\gamma))$ with $dE(\gamma)$ being the Gâteaux derivative of E.

Scattering criticality. Consider the self-consistent hamiltonian

$$h(\rho) := -\Delta + g(\rho), \tag{2.5}$$

Let $f_t(x) := t^{-d} f(\frac{x}{t})$. We say that $g(\rho)$ is *short range* (*scattering subcritical*) if and only if

$$\int_1^\infty \|g(f_t)\|_\infty dt < \infty \tag{2.6}$$

and *long-range* (*scattering critical or supercritical*) otherwise.
Scaling property. Another way to define scattering criticality is to use the *scaling property* of the nonlinearity. Assuming $g(\rho)$ satisfies

$$U_\lambda g(\rho) U_\lambda^{-1} = \lambda^{-\alpha} g(U_\lambda \rho), \tag{2.7}$$

where $U_\lambda : \psi(x) \to \lambda^d \psi(\lambda x)$ and $g(\rho)$ is considered as a multiplication operator and ρ as a function, we say that $g(\rho)$ is scattering subcritical, resp. critical or supercritical, if and only if $\alpha > 1$, resp. $\alpha = 1$ or $\alpha < 1$.

By the way of an example, the scaling property (2.7) holds for $g_1(\rho) = v * \rho$, with the convolution potential $v(x) = \lambda/|x|^\alpha$, for $\alpha < d$, and $v(x) = \lambda\delta(x)$, for $\alpha = d$, and for $g_2(\rho) = \rho^\beta$ with $\alpha = \beta d$.

Thus $g_1(\rho) = \lambda|x|^{-\alpha} * \rho$ and $g_2(\rho) = \rho^\beta$ are subritical (resp. critical, resp. supercritical) iff $\alpha > 1$ and $\beta > 1/d$ (resp. $\alpha = 1$ and $\beta = 1/d$, resp. $\alpha < 1$ and $\beta < 1/d$).

As communicated by Schlein [29] the criticality of $|x|^{-\alpha} * \rho$ and ρ^β are related since $c\rho^{\alpha/d}$ is the semi-classical limit of $|x|^{-\alpha} * \rho$.

Note that if g is scattering sub-critical/critical/supercritical in the scaling sense then it is in the same class in the sense of (2.6). Indeed, if g satisfies (2.7), then

$$g(f_t) = g(U_{\frac{1}{t}}\rho) = t^{-\alpha} U_{\frac{1}{t}} g(\rho) U_{\frac{1}{t}}^{-1},$$

and therefore $\|g(f_t)\|_\infty = t^{-\alpha}\|g(f)\|_\infty$ is integrable at $t = \infty$ iff $\alpha > 1$.

Remark 2.1. For $g(\rho)$ satisfying (2.7) and $g(\lambda\rho) = \lambda^\nu g(\rho)$, (2.7) has scaling covariance with respect to the operator $U_\lambda^\beta := \lambda^{-\beta} U_\lambda$, for an appropriate β.

3. Strategy and main propositions

3.1. **Passing to a Hilbert space.** To work on a Hilbert space, we pass from γ to $\sqrt{\gamma}$, or more precisely to κ, such that $\kappa^*\kappa = \gamma$. One can think of κ as a sort of "half-density". Then the KS (1.1) becomes

$$\partial_t \kappa = i[h(\rho_{\kappa^*\kappa}), \kappa] \tag{3.1}$$

where, recall, $h(\rho) := -\Delta + g(\rho)$, and $\rho_\gamma(x,t) := \gamma(x,x,t)$. Equation (3.1) will be the main focus for our proofs. Note that if $\gamma = \kappa^*\kappa$ is trace-class, then κ is a Hilbert-Schmidt operator.

For brevity, we will use the notation $h_\gamma \equiv h(\rho_\gamma)$ and, for complicated γ, the notation, $\rho(\gamma) \equiv \rho_\gamma$. We have

Proposition 3.1. *Assume* (1.13)-(1.20). *Then* (3.1) $\iff$ (1.1), *in the sense that if* κ *satisfies* (3.1), *then* $\gamma = \kappa^*\kappa$ *is self-adjoint and satisfies* (1.1); *and, in the opposite direction, if* γ *is self-adjoint and satisfies* (1.1), *then* $\gamma = \kappa^*\kappa$, *with* κ *satisfying* (3.1).

Proof. Since γ is assumed to be self-adjoint, ρ_γ and therefore $g(\rho_\gamma)$ are real. Under conditions (1.5)-(1.6), or, more generally, (1.13)-(1.20), the operator h_γ is self-adjoint and therefore generates a unitary evolution which we denote by $U^\gamma(t,s)$. We write $U_t^\gamma \equiv U^\gamma(t,0)$ and $\alpha_t^\gamma(\sigma) := U_t^\gamma \sigma (U_t^\gamma)^{-1}$. (The evolution α_t^γ is generated by the linear operator $\sigma \to [h_\gamma, \sigma]$.) The evolution α_t^γ is differentiable in t on an appropriate dense set (e.g., the non-abelian Sobolev space defined in (4.1)) which is preserved by it and has the following properties:

$$\gamma(t) \text{ satisfies (1.1) with an i.c. } \gamma_0 \iff \gamma(t) = \alpha_t^\gamma(\gamma_0), \tag{3.2}$$

$$\alpha_t^\gamma(\kappa_0^*\kappa_0) = \alpha_t^\gamma(\kappa_0^*)\alpha_t^\gamma(\kappa_0) = \alpha_t^\gamma(\kappa_0)^*\alpha_t^\gamma(\kappa_0). \tag{3.3}$$

If $\kappa(t)$ satisfies (3.1) with an initial condition κ_0, then $\kappa(t) = \alpha_t^\gamma(\kappa_0)$ and therefore by (3.2) and (3.3), $\gamma(t) = \kappa^*(t)\kappa(t) = \alpha_t^\gamma(\kappa_0)^*\alpha_t^\gamma(\kappa_0)$ satisfies (1.1) with the initial condition $\gamma_0 = \kappa_0^*\kappa_0$.

On the other hand, if $\gamma(t)$ satisfies (1.1) with an initial condition $\gamma_0 = \kappa_0^*\kappa_0$, then, by (3.3), $\gamma(t) = \kappa(t)^*\kappa(t)$, where $\kappa(t) := \alpha_t^\gamma(\kappa_0)$ and therefore satisfies $\partial_t\kappa = i[h_\gamma, \kappa]$ (with $\gamma = \kappa^*\kappa$). □

We designate LWP, GWP, AC to stand for 'local well-posedness', 'global well-posedness' and 'asymptotic completeness'. The latter says that for every $\kappa_0 \in W^0$, there exists $\kappa_\infty \in W^0$ such that the solution to (3.1) with the initial condition $\kappa_0 \in W^0$ satisfies

$$\|\kappa(t) - e^{i\Delta t}\kappa_\infty e^{-i\Delta t}\|_{I^2} \to 0. \tag{3.4}$$

Proposition 3.2. *Schematically, we have*

(i) *LWP(κ) $\Rightarrow$ LWP(γ);*
(ii) *GWP(κ) $\Rightarrow$ GWP(γ);*
(iii) *AC(κ) $\Rightarrow$ AC(γ).*

The items (i) and 9ii) follow by $\gamma = \kappa^*\kappa$ using also the uniqueness of trace-class solutions of (1.1). Item (iii) follows from the definitions (1.8) and (3.4) by setting $\gamma_\infty = \kappa_\infty^*\kappa_\infty$.

Theorem 3.3. *The equation* (3.1) *with* (1.13)-(1.20) *and an initial condition* $\kappa_0 = \kappa(t = 0)$ *satisfying, for some integer* $b > d/2$,

$$\big\|\langle\nabla\rangle^b\kappa_0\big\|_{W^0} + \big\|\langle x\rangle^b\kappa_0\big\|_{W^0} \le B < \infty, \tag{3.5}$$

is GWP and AC.

The proof of Theorem 3.3 is given after Theorem 3.6 below. Theorem 1.1 follows from Theorem 3.3 and Proposition 3.2.

Remark 3.4. (1) Unlike (1.1), Eq (3.1) has a *gauge symmetry*: for any unitary operator U, which commutes with h_ρ (i.e. is a symmetry of h_ρ), if κ is a solution to (3.1), then so is $U\kappa$. Note that $U\kappa$ produces the same γ as κ: $(U\kappa)^*U\kappa = \kappa^*\kappa$.

(2) The nonlinearity $\hat g(\kappa) := [g(\rho_{\kappa^*\kappa}), \kappa]$ inherits the gauge symmetry very important for our analysis:

$$e^{i\chi}\hat g(\kappa)e^{-i\chi} = \hat g(e^{i\chi}\kappa e^{-i\chi}) \tag{3.6}$$

for any differentiable function χ. To see this it suffices to observe that $e^{i\chi}\rho_\gamma e^{-i\chi} = \rho_\gamma = \rho(e^{i\chi}\gamma e^{-i\chi})$.

(3) (I. Chenn) In the time-dependent case, the following equation

$$\partial_t\kappa = ih_{\kappa^*\kappa}\kappa \tag{3.7}$$

also leads to (1.1), if $\gamma = \kappa^*\kappa$, however it does not give the time-independent equation corresponding to (1.1).

3.2. **Local decay for κ and main propositions.** At the heart of understanding the long-time behaviour of solutions is the *local decay* property which shows that, as time progresses, solutions move out of bounded regions of the physical space and quantifies how quickly this happens. It is usually stated as a bound on a local norm, i.e. a norm measuring concentration of the solution in bounded domains. If such a bound is sufficiently strong, it implies the global existence and scattering property.

To formulate precisely a local decay result for the Hilbert-Schmidt operator κ, with an integral kernel $\kappa(x, y)$, we introduce the local norms

$$\|\kappa\|_{L^q_r L^p_c} \equiv \|\tilde\kappa\|_{L^q_r L^p_c} := \|\|\tilde\kappa\|_{L^p_c}\|_{L^q_r}. \tag{3.8}$$

for $1 \le p, q \le \infty$, where $\tilde\kappa(r, c)$ is the kernel given by

$$\tilde\kappa(r, c) := \kappa(x, y), \qquad \text{where} \quad r := y - x, \quad c := \frac{1}{2}(y + x). \tag{3.9}$$

Definition 1. We say that $\kappa(t)$ satisfies the *local decay* property $\mathrm{LD}_\nu(\kappa)$ if $\|\kappa(t)\|_{L^2_r L^s_c} \lesssim t^{-\nu}$ for $\nu = d(1/2 - 1/s)$ and some $s > 2$.

Proposition 3.5. *With the notation* LD_ν *above (in addition to the notation LWP, GWP, AC introduced in the paragraph preceding Proposition 3.2), we have, if* $\nu > 1$,

$$LWP(\kappa) + LD_\nu(\kappa) \quad\Longrightarrow\quad GWP(\kappa) + AC(\kappa). \tag{3.10}$$

The proof of (3.10) is given in Section 8 and relies on standard arguments. Proposition 3.5 reduces the proof of Theorem 3.3 to the proof of $\mathrm{LD}_\nu(\kappa)$ (LWP is standard and given by Theorem 8.1) to which we proceed.

In what follows, the exponent α appearing in several interpolation type inequalities is always assumed to satisfy the condition

$$\alpha \geq 0 \quad \text{and} \quad \alpha < 1 \text{ for } d \text{ even}, \quad \alpha \leq 1 \text{ for } d \text{ odd}. \tag{3.11}$$

Here is the key local decay result for Eq (3.1):

Theorem 3.6 (Local decay)**.** *Assume $d \leq 3$ and conditions* (1.13)-(1.20). *Let κ be the local-in-time solution of* (3.1) *(see Theorem 8.1), with initial datum $\kappa(t=0) =: \kappa_0$ satisfying* (3.5). *Then there exists $\lambda_0 = \lambda_0(B) > 0$ small enough such that for all $|\lambda_1|, |\lambda_2| \leq \lambda_0$ we have*

$$\|\kappa\|_{L^2_r L^s_c} \lesssim |t|^{-\alpha b} \|\langle x\rangle^b \kappa_0\|^\alpha_{W^0} \|\kappa_0\|^{1-\alpha}_{W^0}, \tag{3.12}$$

$$\alpha b = d(\frac{1}{2} - \frac{1}{s}), \quad 2 \leq s \leq \infty. \tag{3.13}$$

Proof of Theorem 3.3. A local-in-time solution to (3.1), under the conditions stated in Theorem 3.6, is provided by the local existence Theorem 8.1.

The global existence and scattering for (3.1) follow from the local existence Theorem 8.1, the local decay from Theorem 3.6 and Proposition 3.5. ☐

The proof of Theorem 3.6 will follow from a non-commutative version of a weighted Gagliardo-Nirenberg-Klainerman-type interpolation inequality (Proposition 3.7) and an a priori energy estimate in the weighted space W^b (Proposition 3.8).

Proposition 3.7. *For any $s \geq 2$ and $\alpha \in [0,1)$ for d even, $\alpha \in [0,1]$ for d odd, we have*

$$\|\kappa(t)\|_{L^2_r L^s_c} \lesssim |t|^{-\alpha b} \|\kappa(t)\|^\alpha_{W^b} \|\kappa(t)\|^{1-\alpha}_{W^0}, \qquad \alpha b = d(\frac{1}{2} - \frac{1}{s}). \tag{3.14}$$

This proposition is proven in Section 4. The next result gives a priori energy inequalities.

Proposition 3.8 (A priori bounds)**.** *Assume $d \leq 3$. Let $b > d/2$ be an integer, and λ_1, λ_2 denote the coupling constants in* (1.13). *There exists an absolute constant c_0 such that, any solution κ to equation* (3.1) *which satisfies for some time $s \geq 0$,*

$$|\lambda_1| \|\kappa(s)\|^2_{W^b} + |\lambda_2| \|\kappa(s)\|^{2\beta}_{W^b} < \frac{c_0}{2^{\max\{3, 2\beta+1\}}}, \tag{3.15}$$

also satisfies for any $t > s$

$$\|\kappa(t)\|_{W^b} \leq 2\|\kappa(s)\|_{W^b}. \tag{3.16}$$

Remark 3.9. We do not need a smallness condition $|\lambda_1|, |\lambda_2| \ll 1$ in Theorem 3.6 if we start at a sufficiently large time t_0. We can then solve the final state problem in our setting without assuming weakly nonlinear interactions.

Proposition 3.8 is proven in Section 7. The main idea here is to use that the Galilean boost observable J is almost conserved under (3.1), see Proposition 6.1. We remark that the *gauge invariance* (3.6) of the nonlinearity, and more precisely the invariance of (3.1) under the Galilean transformations (1.24) plays an important role in this proof.

Remark 3.10. The following lemma used in the proof of the local decay for γ and Lemma 7.1 below establishes a relation between local rc- and xy-norms:

Lemma 3.11. *For all $s \geq 2$ we have*

$$\|\kappa\|_{L^s_x L^2_y} \leq \|\kappa\|_{L^2_r L^s_c}, \quad \text{where } \|\kappa\|_{L^s_x L^2_y} := \big\| \|\kappa(x,y)\|_{L^2_y} \big\|_{L^s_x}. \tag{3.17}$$

Proof. Recall the notation (3.9) and introduce the function

$$f(x) := \|\kappa\|^2_{L^2_y}(x) = \int |\kappa(x,y)|^2 dy = \int |\tilde{\kappa}(r, x - r/2)|^2 dr. \tag{3.18}$$

Then $\|\kappa\|^2_{L^s_x L^2_y} = \|f\|_{L^{s/2}} \leq \int \big\| |\tilde{\kappa}(r, x - r/2)|^2 \big\|_{L^{s/2}_x} dr = \int \big\| \tilde{\kappa}(r, \cdot) \big\|^2_{L^s_c} dr = \|\tilde{\kappa}\|^2_{L^2_r L^s_c}$. $\square$

Local decay for γ. We end this section by discussing local decay for $\gamma = \kappa^* \kappa$, which is of independent interest, although it is not used in the proof of Theorem 1.1.

Definition 2 (Local norms for γ)**.** We define the local norm of operators γ through their integral kernels $\gamma(x,y)$ as

$$\|\gamma\|_{(s)} := \left(\int_{\mathbb{R}^d \times \mathbb{R}^d} |\gamma(x,y)|^s \, dx dy \right)^{1/s}, \tag{3.19}$$

with the standard adjustment for $s = \infty$.

Note that

$$\|\gamma\|_{(s)} \leq \|\kappa\|^2_{L^s_x L^2_y}, \qquad \|\kappa\|_{L^s_x L^2_y} := \big\| \|\kappa(x,y)\|_{L^2_y} \big\|_{L^s_x} \tag{3.20}$$

Now, (3.20), (3.17), and Theorem 3.6 imply that the solutions of (1.1) described in Theorem 1.1 have the following local decay property: for all $t \in \mathbb{R}$,

$$\|\gamma(t)\|_{(s)} \lesssim |t|^{-d(1-2/s)}, \qquad 2 \leq s \leq \infty. \tag{3.21}$$

4. Proof of Proposition 3.7

The main idea here is first to extend the Gagliardo-Nirenberg inequality to the non-abelian Sobolev-type spaces

$$V^s := \Big\{ \kappa \in I^2 \, : \, \sum_{|\alpha| \leq s} \|D^\alpha \kappa\|_{I^2} < \infty \Big\}, \tag{4.1}$$

for any $s \geq 0$, with the grading provided by the commutators

$$D_\ell \kappa := [\partial_{x_\ell}, \kappa], \qquad D = (D_1, \ldots, D_d) = [\nabla, \cdot], \tag{4.2}$$

and then observe that the commutator vector-field defined in (1.12) is related to D by the formula

$$J_t = -2it U_t^* D U_t, \tag{4.3}$$

where $U_t : \psi(x) \to e^{-ix^2/4t} \psi(x)$.

Another important observation used in the proof is that, if we denote the map from operators κ to their transformed kernes $\tilde{\kappa}(r,c)$ by ϕ, then we have

$$\phi(D_i \kappa) = \partial_{c_i} \phi(\kappa). \tag{4.4}$$

Passing from operators κ to the integral kernels $\tilde\kappa(r,c) := \kappa(x,y)$, where $r := y - x,\ c := \frac{1}{2}(y+x)$ (see (3.9)) and applying the standard Gagliardo-Nirenberg interpolation inequality in the c-variable, we find

$$\|\tilde\kappa\|_{L^s_c} \lesssim \|\partial^b\tilde\kappa\|^{\alpha}_{L^2_c}\|\tilde\kappa\|^{1-\alpha}_{L^2_c}, \tag{4.5}$$

$$b\alpha = d(\frac{1}{2} - \frac{1}{s}),\ s \geq 2, \tag{4.6}$$

and $0 \leq \alpha < 1$ for d even and $0 \leq \alpha \leq 1$ for d odd. Applying to this the Hölder inequality with the exponents $1/\alpha$ and $1/(1-\alpha)$, we obtain furthermore

$$\|\tilde\kappa\|_{L^2_rL^s_c} \lesssim \|\partial^b\tilde\kappa\|^{\alpha}_{L^2_rL^2_c}\|\tilde\kappa\|^{1-\alpha}_{L^2_rL^2_c}. \tag{4.7}$$

Next, we claim that

$$\|\partial^b\tilde\kappa\|_{L^2_rL^2_c} = \|D^b\kappa\|_{I^2}. \tag{4.8}$$

Indeed, we use (4.4) to define $D^r_i\kappa$, for arbitrary positive powers of derivatives, by $\phi(D^r_i\kappa) := \partial^r_{c_i}\phi(\kappa)$, where $\partial^r_{c_i}$ is the standard fractional derivative, see for example [32]. Since $\|\tilde\kappa\|_{L^2_rL^2_c} = \|\kappa\|_{I^2}$, (4.8) follows. Relations (4.7), (4.8) and (4.4) imply

$$\|\kappa(t)\|_{L^2_rL^s_c} \lesssim \|D^b\kappa(t)\|^{\alpha}_{I^2}\|\kappa(t)\|^{1-\alpha}_{I^2}, \tag{4.9}$$

with (4.6), which gives the non-abelian Gagliardo-Nirenberg inequality. Now, using (4.3) and the relation $I^2 = W^0$, we convert this into

$$\|\kappa(t)\|_{L^2_rL^s_c} \lesssim |t|^{-\alpha b}\|J^b\kappa(t)\|^{\alpha}_{W^0}\|\kappa(t)\|^{1-\alpha}_{W^0}, \tag{4.10}$$

with (4.6), b positive integer and $\alpha \in [0,1]$ satisfying (3.11), which is a stronger (scale-invariant) version of (3.14). □

5. Local norm and density estimates

As a preparation for demonstrating Proposition 3.8, we prove several inequalities on local norms and densities.

Lemma 5.1 (Estimates on the density)**.** *Let $1/w + 1/w' = 1/q$. Then*

$$\|\rho(\kappa\kappa')\|_q \lesssim \|\kappa\|_{L^2_rL^w_c}\|\kappa'\|_{L^2_rL^{w'}_c}. \tag{5.1}$$

Proof. Using that $\rho(\kappa\kappa') = \int \kappa(x,y)\kappa'(y,x)dy$ and passing from κ to $\tilde\kappa$, we find

$$\begin{aligned}
\|\rho(\kappa\kappa')\|_q &= \|\int \tilde\kappa(x-y, \frac{1}{2}(x+y))\tilde{\kappa'}(x-y, \frac{1}{2}(x+y))dy\|_{L^q_x} \\
&= \|\int \tilde\kappa(r, x - \frac{1}{2}r)\tilde{\kappa'}(r, x - \frac{1}{2}r)dr\|_{L^q_x} \\
&\lesssim \int \|\tilde\kappa(r, x - \frac{1}{2}r)\tilde{\kappa'}(r, x - \frac{1}{2}r)\|_{L^q_x}dr \\
&= \int \|\tilde\kappa(r,c)\tilde{\kappa'}(r,c)\|_{L^q_c}dr \\
&\lesssim \int \|\tilde\kappa\|_{L^w_c}\|\tilde{\kappa'}\|_{L^{w'}_c}dr.
\end{aligned} \tag{5.2}$$

Upon application of the Schwarz inequality, this yields (5.1). □

Now, applying (3.14) gives

Corollary 5.2. *Let $q \geq 1$, $\alpha, \alpha' \in [0,1]$ satisfy (3.11) and $\nu := \alpha b + \alpha' b' = d(1 - \frac{1}{q})$. Then*

$$\|\rho(\kappa\kappa')\|_q \lesssim |t|^{-\nu} \|\kappa\|_{W^b}^{\alpha} \|\kappa\|_{W^0}^{1-\alpha} \|\kappa'\|_{W^{b'}}^{\alpha'} \|\kappa'\|_{W^0}^{1-\alpha'}. \tag{5.3}$$

Next, we have

Lemma 5.3 (Products of functions and half-densities)**.** *Let f be a multiplication operator by $f \in L^p$. Then*

$$\|f\kappa\|_{W^0} \lesssim \|f\|_{L^p} \|\kappa\|_{L^2_r L^s_c} \tag{5.4}$$

$$\lesssim |t|^{-\alpha b} \|f\|_p \|J^b \kappa\|_{W^0}^{\alpha} \|\kappa\|_{W^0}^{1-\alpha}, \tag{5.5}$$

where $\alpha b = d/p$ and $1/p + 1/s = 1/2$.

Proof. Let $p^{-1} + s^{-1} = \frac{1}{2}$. We estimate

$$\begin{aligned} \|f\kappa\|_{W^0}^2 &= \iint |f(x)\kappa(x,y)|^2 dxdy \\ &= \iint |f(c + \frac{1}{2}r)\tilde{\kappa}(r,c)|^2 drdc \\ &\leq \int \|f\|_{L^p}^2 \|\tilde{\kappa}\|_{L^s_c}^2 dr = \|f\|_{L^p}^2 \|\tilde{\kappa}\|_{L^2_r L^s_c}^2. \end{aligned}$$

This gives (5.4). The latter and (3.14) imply (5.5). □

Next, we prove the following elementary inequality

$$\left|\rho_{J(\kappa^*\kappa)}(x)\right|^2 \leq 2\rho_{J\kappa^* J\kappa}(x)\rho_{\kappa^*\kappa}(x). \tag{5.6}$$

To prove this, we use $J(\kappa^*\kappa) = (J\kappa^*)\kappa + \kappa^*(J\kappa)$ to estimate

$$\begin{aligned} &\left|\rho_{J(\kappa^*\kappa)}(x)\right|^2 \leq 2(\int_{\mathbb{R}^3} \left|\overline{J\kappa(z,x)}\kappa(z,x)\right| dz)^2 \\ &\leq 2\int_{\mathbb{R}^3} |J\kappa(z,x)|^2 dz \int_{\mathbb{R}^3} |\kappa(z,x)|^2 dz \end{aligned}$$

which implies the inequality (5.6).

6. Approximate Galilean conservation law

In this section we prove energy-type inequalities for 'half-densities' κ. The first lemma is related to the invariance of (1.1) and (3.1) under Galilean transformations (1.24). In what follows, we use the following relation (which we call Jacobi-Leibniz rule)

$$J[a,b] = [Ja,b] + [a,Jb], \tag{6.1}$$

which follows from the Jacobi identity $[[A,B],C] + [[C,A],B] + [[B,C],A] = 0$.

Proposition 6.1 (Galilean invariance)**.** *Denote $D_\gamma\kappa := \partial_t\kappa - i[h_\gamma, \kappa]$. Then D_γ and J almost commute in the sense that*

$$D_\gamma J\kappa = JD_\gamma\kappa + i[dg(\rho_\gamma)\rho_{J\gamma}, \kappa]. \tag{6.2}$$

Moreover, if we let $J^2 = J_{\ell_2}J_{\ell_1}$, for any $\ell_1, \ell_2 = 1, \dots d$, then we have

$$\begin{aligned} D_\gamma J^2\kappa &= J^2 D_\gamma\kappa + i[dg(\rho_\gamma)\rho_{J^2\gamma}, \kappa] \\ &\quad + i[d^2g(\rho_\gamma)\rho_{J_{\ell_1}\gamma}\rho_{J_{\ell_2}\gamma}, \kappa] + i[dg(\rho_\gamma)\rho_{J_{\ell_2}\gamma}, J_{\ell_1}\kappa] + i[dg(\rho_\gamma)\rho_{J_{\ell_1}\gamma}, J_{\ell_2}\kappa], \end{aligned} \tag{6.3}$$

where, recall, d^kg is the k-th Gâteaux derivative of g.

Proof. First, we compute

$$[j, \partial_t\kappa] = \partial_t[j, \kappa] + 2[p, \kappa]. \tag{6.4}$$

This, together with (6.1), implies

$$[j, [h_0, \kappa]] = [[j, h_0], \kappa] + [h_0, [j, \kappa]] = [h_0, [j, \kappa]] - 2i[p, \kappa]. \tag{6.5}$$

Subtracting (6.5) times i from (6.4) we obtain $[j, \partial_t\kappa - i[h_0, \kappa]] = \partial_t[j, \kappa] - i[h_0, [j, \kappa]]$, which can be rewritten as

$$JD_0 = D_0J, \qquad D_0\kappa := \partial_t\kappa - i[h_0, \kappa]. \tag{6.6}$$

To deal with the difference $(D_\gamma - D_0)\kappa = -i[g(\rho_\gamma), \kappa]$ we use that g is covariant under translations and gauge transformations and therefore it is also covariant under the Galilean transformations (1.24).

For a general nonlinearity $f(\gamma)$, the covariance relation states $U_{v,t}f(\gamma)U^*_{v,t} = f(U_{v,t}\gamma U^*_{v,t})$. Differentiating it with respect to v at $v = 0$, we find

$$[j, f(\gamma)] = df(\gamma)[j, \gamma]. \tag{6.7}$$

Taking here $f(\gamma) = g(\rho_\gamma)$ and using that $df(\gamma)\xi = dg(\rho_\gamma)d\rho_\gamma\xi$ and $d\rho_\gamma\xi = \rho_\xi$, this gives

$$[j, g(\rho_\gamma)] = dg(\rho_\gamma)\rho_{[j,\gamma]}, \tag{6.8}$$

which, together with the Jacobi-Leibnitz identity (6.1), yields

$$J[g(\rho_\gamma), \kappa] = [Jg(\rho_\gamma), \kappa] + [g(\rho_\gamma), J\kappa]. \tag{6.9}$$

We combine (6.6) and (6.8)-(6.9) to obtain

$$JD_\gamma\kappa = D_\gamma J\kappa - i[dg(\rho_\gamma)\rho_{J\gamma}, \kappa]. \tag{6.10}$$

which is (6.2).

To prove (6.3), we recall $J^2 = J_{\ell_2}J_{\ell_1}$ and iterate (6.10). On the first step, we have

$$J^2D_\gamma\kappa = J_{\ell_2}D_\gamma J_{\ell_1}\kappa - iJ_{\ell_2}[dg(\rho_\gamma)\rho_{J_{\ell_1}\gamma}, \kappa] \tag{6.11}$$

Now, using (6.10) again, we find for the first term on the right-hand side

$$J_{\ell_2}D_\gamma J_{\ell_1}\kappa = D_\gamma J^2\kappa - i[dg(\rho_\gamma)\rho_{J_{\ell_2}\gamma}, J_{\ell_1}\kappa] \tag{6.12}$$

For the second term on the right-hand side of (6.11), we use relation (6.1) to find

$$\begin{aligned} J_{\ell_2}[dg(\rho_\gamma)\rho_{J_{\ell_1}\gamma}, \kappa] &= [d^2g(\rho_\gamma)\rho_{J_{\ell_2}\gamma}\rho_{J_{\ell_1}\gamma} + dg(\rho_\gamma)\rho_{J_{\ell_2}J_{\ell_1}\gamma}, \kappa] \\ &\quad + [dg(\rho_\gamma)\rho_{J_{\ell_1}\gamma}, J_{\ell_2}\kappa]. \end{aligned} \tag{6.13}$$

Combining (6.11), (6.12) and (6.13) gives (6.3). □

With J as defined in (1.12), let us denote

$$J^m = \prod_{i=1}^{d} J_i^{m_i}, \qquad m = (m_1, \dots, m_d). \tag{6.14}$$

Using the key relation (6.2) we derive the following identity for the evolution of the weighted energy:

Lemma 6.2 (Evolution of the weighted energy)**.** *Assume* κ *satisfies* (3.1)*. Then*

$$\frac{1}{2}\partial_t \|J^m \kappa\|_{W^0}^2 = \mathrm{Im}\langle J^m\kappa, R_m\rangle_{W^0}, \tag{6.15}$$

with

$$\begin{aligned} R_m &:= \sum_{k=1}^{|m|} \sum_a c_{k,m} [d^k g(\rho_\gamma) \prod_{i=1}^{k} \rho_{J^{s_i}\gamma}, J^a \kappa], \\ &\sum_{i=1}^{k} s_i + |a| = |m|, \quad s_i > 0, \quad (|a| \le |m| - 1), \end{aligned} \tag{6.16}$$

for some constants $c_{k,m}$*. Here* $\langle \kappa, \kappa' \rangle_{W^0}$ *is the* $W^0 = I^2$ *inner product defined in* (1.10)*.*

Proof. For simplicity, we show (6.15)–(6.16) only in the $|m| = 1, 2$ cases, which is sufficient to do our a priori estimates in dimensions $d \le 3$. It will be clear to the reader how this generalizes applying the arguments below and Faá-di Bruno's formula.

We compute $\partial_t \|J^m\kappa\|_{W^0}^2 = 2\,\mathrm{Re}\langle J^m\kappa, \partial_t J^m \kappa\rangle_{W^0}$. Now, using $\partial_t \kappa' = D_\gamma \kappa' + i[h_\gamma, \kappa']$ with $\kappa' = J^m\kappa$ and $\mathrm{Re}\langle J^m\kappa, i[h_\gamma, J^m\kappa]\rangle_{W^0} = 0$ yields

$$\partial_t \|J^m\kappa\|_{W^0}^2 = 2\,\mathrm{Re}\langle J^m\kappa, D_\gamma J^m\kappa\rangle_{W^0}. \tag{6.17}$$

Now, letting $|m| = 1$ and applying (6.2) with $\gamma = \kappa^*\kappa$ and $D_\gamma\kappa = 0$ (by (3.1)) gives

$$\frac{1}{2}\partial_t \|J_\ell \kappa\|_{W^0}^2 = \mathrm{Re}\langle J_\ell\kappa, i[dg(\rho_\gamma)\rho_{J_\ell\gamma}, \kappa]\rangle_{W^0}, \tag{6.18}$$

which gives (6.15)–(6.16) with $|m| = 1$.

To compute in the case $|m| = 2$, we begin with (6.17) with $|m| = 2$ and simplify our notation by denoting $J^2 = J_{\ell_2}J_{\ell_1}$, for any $\ell_1, \ell_2 = 1, \dots d$. To compute the right-hand side of (6.17), we plug (6.3) into (6.17) with $|m| = 2$ and $\gamma = \kappa^*\kappa$, and using $D_\gamma\kappa = 0$ (by (3.1)) to obtain

$$\begin{aligned} \frac{1}{2}\partial_t \|J^2\kappa\|_{W^0}^2 = \mathrm{Im}\langle J^2\kappa, &[dg(\rho_\gamma)\rho_{J^2\gamma}, \kappa] + [d^2 g(\rho_\gamma)\rho_{J_{\ell_1}\gamma}\rho_{J_{\ell_2}\gamma}, \kappa] \\ &+ [dg(\rho_\gamma)\rho_{J_{\ell_2}\gamma}, J_{\ell_1}\kappa] + [dg(\rho_\gamma)\rho_{J_{\ell_1}\gamma}, J_{\ell_2}\kappa]\rangle_{W^0}, \end{aligned}$$

which is of the form (6.15)–(6.16) with $|m| = 2$. $\square$

7. Proof of Proposition 3.8

This is our main lemma on the control of the evolution of the weighted energy:

Lemma 7.1. *Assume* (1.13)-(1.20) *and* $d \leq 3$ *and let* $\kappa(t)$ *satisfy* (3.1) *with a self-interaction* g *as in* (1.13). *Then, for* $b = [d/2] + 1$, *there exists an absolute constant* C_0 *such that*

$$\Big|\frac{d}{dt}\|\kappa(t)\|_{W^b}\Big| \leq C_0|\lambda_1|\,|t|^{-d(1+\frac{1}{p}-\frac{1}{q})}\|\kappa(t)\|_{W^0}\|\kappa(t)\|^2_{W^b} + C_0|\lambda_2|\,|t|^{-d\beta}\|\kappa(t)\|^{2\beta+1}_{W^b}, \tag{7.1}$$

where (p, q) *is an admissible pair from conditions* (1.16)–(1.17), *and* β *is the exponent in* (1.21).

This statement holds in $d \geq 4$ as well by appropriately modifying the assumptions (1.14)-(1.21), see Remarks 1.3 and 7.2. The constant C_0 appearing in (7.1) determines the constant c_0 in (3.15) as $c_0 := C_0^{-1}$. Before proving Lemma 7.1 let us show how it implies the main Proposition 3.8.

Proof of Propositions 3.8. Integrating inequality (7.1) and using that $d(1 + \frac{1}{p} - \frac{1}{q}) > 1$, by (1.18), and $d\beta > 1$ by (1.21), we obtain

$$\Big|\|\kappa(t)\|_{W^b} - \|\kappa(s)\|_{W^b}\Big| \leq C_0 \sup_{s\leq r\leq t}\big(|\lambda_1|\|\kappa(r)\|_{W^0}\|\kappa(r)\|^2_{W^b} + |\lambda_2|\|\kappa(r)\|^{2\beta+1}_{W^b}\big). \tag{7.2}$$

Letting $A(t) := \sup_{s\leq r\leq t}\|\kappa(r)\|_{W^b}$, (7.2) gives

$$A(t) \leq A(s) + C_0\big(|\lambda_1|A(t)^3 + |\lambda_2|A(t)^{2\beta+1}\big). \tag{7.3}$$

For fixed time s as in the statement, see (3.15), let us consider the set of times

$$\mathcal{T} := \{t \in [s, \infty) \,:\, A(t) \leq 2A(s)\}. \tag{7.4}$$

$\mathcal{T}$ is non-empty and closed by definition, since from Theorem 8.1(iii) we know that $A(t)$ is a continuous function (for proper solutions κ). Moreover, if $s < t \in \mathcal{T}$, then from (7.3) and assumption (3.15) with $c_0 = C_0^{-1}$ we get

$$A(t) \leq A(s) + 2^{\max\{3,2\beta+1\}}C_0\big(|\lambda_1|A(s)^3 + |\lambda_2|A(s)^{2\beta+1}\big) < 2A(s).$$

Thus, by continuity, there exists $\delta > 0$ such that $A(t') \leq 2A(s)$ for $|t' - t| < \delta$. It follows that $\mathcal{T}$ is open and therefore $\mathcal{T} = [s, \infty)$, which is the desired statement (3.16). □

Proof of Lemma 7.1. The starting point is (6.15). To estimate the right-hand side of (6.15) for $|m| = 1, 2$, we use the non-commutative Schwarz inequality to obtain

$$\begin{aligned}&|\langle J^m\kappa, [d^k g(\rho_\gamma)(\rho_{J^s\gamma})^k, J^a\kappa]\rangle_{W^0}|\\ &\lesssim \|J^m\kappa\|_{W^0}\|[d^k g(\rho_\gamma)(\rho_{J^s\gamma})^k, J^a\kappa]\|_{W^0},\end{aligned} \tag{7.5}$$

where

$$1 \leq k \leq |m|, \quad |s| \geq 1, \quad |s|k + |a| = |m|, \quad |m| = 1, 2. \tag{7.6}$$

Now, we claim the following estimates: for parameters as in (7.6) we have

$$\|[d^k g_i(\rho_\gamma)(\rho_{J^s\gamma})^k, J^a\kappa]\|_{W^0} \lesssim t^{-\nu_i}\|\kappa\|^{p_i}_{W^m}, \qquad i = 1, 2, \tag{7.7}$$

where, recall, g_i are the components of g in (1.13) satisfying (1.18) and

$$\begin{aligned} &\nu_1 = d(1 + 1/p - 1/q), \qquad p_1 = 3, \\ &\nu_2 = \beta d, \qquad p_2 = 2\beta + 1. \end{aligned} \tag{7.8}$$

Estimates for g_1. We begin with $k = 1$. (5.5) and (5.3) (with $\alpha = \alpha' = 1$), together with the relation $\rho_{J(\kappa^*\kappa)} = \rho_{J(\kappa^*)\kappa} + \rho_{\kappa^* J(\kappa)}$ and assumption (1.15), give

$$\begin{aligned} \|[dg_1(\rho_\gamma)\rho_{J^s\gamma}, J^a\kappa]\|_{W^0} &\lesssim t^{-b}\|dg_1(\rho_\gamma)\rho_{J^s\gamma}\|_p\|J^{b+a}\kappa\|_{W^0} \\ &\lesssim t^{-b}\|\rho_{J^s\gamma}\|_q\|\kappa\|_{W^{b+a}} \\ &\lesssim t^{-b-\nu}\|\kappa\|_{W^{b'+s'}}\|\kappa\|_{W^{b''+s''}}\|\kappa\|_{W^{b+a}}, \end{aligned} \tag{7.9}$$

where $s' + s'' = |s|$, $\nu := d(1 - \frac{1}{q})$, $b = d/p$, and b' and b'' are any non-negative numbers satisfying $b' + b'' = d(1 - \frac{1}{q})$. Since $d(1 - \frac{1}{q}) \le |m|$ and $|s| + |a| = |m|$, we can choose s', s'', b', b'', a so that $b' + s', b'' + s'', b + |a| \le |m|$. Since $\nu + b = d(1 + 1/p - 1/q)$, this gives

$$\|[dg_1(\rho_\gamma)\rho_{J^s\gamma}, J^a\kappa]\|_{W^0} \lesssim t^{-d(1+\frac{1}{p}-\frac{1}{q})}\|\kappa\|^3_{W^m}, \tag{7.10}$$

$$d(1 - \frac{1}{q}) \le |m|, \quad |s| + |a| = |m|. \tag{7.11}$$

The latter conditions imply that $d(1+1/p-1/q)+|a| \le 2|m|$. Since $d(1+1/p-1/q) > 1$ this gives $1 + |a| < 2|m|$. Equation (7.10) then gives (7.7) for $i = 1$ and $|m| = k = |s| = 1, a = 0$ and $|m| = 2, k = 1, |s| + |a| = 2$.

Now, we prove (7.7) for $i = 1$ and $|k| = 2$, which implies $2|s| + |a| = |m|$. We use the assumption (1.16) instead of (1.15) to obtain, for $a = 0$, as in (7.9),

$$\begin{aligned} \|[d^2g_1(\rho_\gamma)(\rho_{J^s\gamma})^2, \kappa']\|_{W^0} &\lesssim t^{-b}\|d^2g_1(\rho_\gamma)(\rho_{J^s\gamma})^2\|_p\|J^b\kappa'\|_{W^0} \\ &\lesssim t^{-b}\|\rho_{J^s\gamma}\|^2_{q'}\|J^b\kappa\|_{W^0} \\ &\lesssim t^{-b-2\nu}\|J^{b'+s'}\kappa\|^2_{W^0}\|J^{b''+s''}\kappa\|^2_{W^0}\|J^b\kappa'\|_{W^0}, \end{aligned} \tag{7.12}$$

where $s' + s'' = s$, $\nu := d(1 - \frac{1}{q'})$, $b = d/p$, and b' and b'' are any non-negative numbers satisfying $b' + b'' = d(1 - \frac{1}{q'})$. Since $d(1 - \frac{1}{q'}) \le |m|$ and $|s| + |a| \le |m|$, we can choose them so that $b' + s', b'' + s'' \le |m|$, giving

$$\|[d^2g_1(\rho_\gamma)(\rho_{J^s\gamma})^2, \kappa']\|_{W^0} \lesssim t^{-d(2-\frac{2}{q'}+\frac{1}{p})}\|\kappa\|^4_{W^m}\|\kappa'\|_{W^m}. \tag{7.13}$$

This completes the proof of (7.7) for $i = 1$ and $k = 2$ and $a = 0$, which suffices for $|m| = 2$.

Estimates for g_2. As above, we rely on the inequality (3.14), but now need a different argument for the estimates in view of the possible singular nature of the derivatives of the exchange-correlation term ρ^β.

We prove (7.7) for $i = 2$ and $|m| = k = 1$ which implies $|s| = 1, a = 0$. To this end, we need to estimate $\|[dg_2(\rho_\gamma)(\rho_{J\gamma}), \kappa]\|_{W^0}$. We calculate explicitly

$$\begin{aligned}\|dg_2(\rho_\gamma)(\rho_{J\gamma})\,\kappa\|_{W^0}^2 &= \beta^2 \int_{\mathbb{R}^3\times\mathbb{R}^3} \left|\rho_\gamma^{\beta-1}(x)\,\rho_{J\gamma}(x)\,\kappa(x,y)\right|^2 dxdy\\ &= \beta^2 \int_{\mathbb{R}^3} \rho_\gamma^{2\beta-2}(x)\,\rho_{J\gamma}^2(x)\,(\int_{\mathbb{R}^3} |\kappa(x,y)|^2 dy)dx\\ &= \beta^2 \int_{\mathbb{R}^3} \rho_\gamma^{2\beta-1}(x)\,\rho_{J\gamma}^2(x)\,dx. \end{aligned}\tag{7.14}$$

Now, using the relations $\gamma = \kappa^*\kappa$ and (5.6) in (7.14), $\rho_{\kappa^*\kappa} = \|\kappa\|_{L^2_y}^2$, and $\|\kappa\|_{L^\infty_x L^2_y} \lesssim \|\kappa\|_{L^2_r L^\infty_c}$, we find

$$\begin{aligned}\|dg_2(\rho_\gamma)(\rho_{J\gamma})\,\kappa\|_{W^0}^2 &\le 2\beta^2 \int_{\mathbb{R}^3} \rho_{\kappa^*\kappa}^{2\beta}(x)\,\rho_{J\kappa^*J\kappa}(x)\,dx\\ &\le 2\beta^2 \|\kappa\|_{L^2_r L^\infty_c}^{4\beta} \|J\kappa\|_{L^2_x L^2_y}^2. \end{aligned}\tag{7.15}$$

The second factor on the right-hand side of (7.15) is equal $\|J\kappa\|_{W^0}^2$. For the first factor, we use (3.14) with $s = \infty$ and $\alpha = 1$ to find, for $b = [d/2] + 1$,

$$\|dg_2(\rho_\gamma)(\rho_{J\gamma})\,\kappa\|_{W^0} \lesssim t^{-\beta d} \|\kappa\|_{W^b}^{2\beta} \|J\kappa\|_{W^0},\tag{7.16}$$

which yields (7.7) for $|m| = 1$.

We now consider (7.7) with $|m| = 2$ and $k = 1, a = 0$ and $|s| = 2$. We compute as in (7.14)

$$\begin{aligned}\|dg_2(\rho_\gamma)\rho_{J^s\gamma}\,\kappa\|_{W^0}^2 &= \beta^2 \int_{\mathbb{R}^3} \rho_\gamma^{2\beta-2}(x)\,\rho_{J^s\gamma}^2(x)\,(\int_{\mathbb{R}^3} |\kappa(x,y)|^2 dy)dx\\ &= \beta^2 \int_{\mathbb{R}^3} \rho_\gamma^{2\beta-1}(x)\,\rho_{J^s\gamma}^2(x)\,dx. \end{aligned}\tag{7.17}$$

Using the relation $J^2(\kappa^*\kappa) = (J^2\kappa^*)\kappa + \kappa^*(J^2\kappa) + 2(J\kappa^*)J\kappa)$ in (7.17), and $\beta \ge 1/2$, we find

$$\|dg_2(\rho_\gamma)\rho_{J^s\gamma}\,\kappa\|_{W^0} \lesssim \|J^s\kappa\|_{L^2_x L^2_y} \|\kappa\|_{L^2_r L^\infty_c}^{2\beta}\tag{7.18}$$

$$+\, \|\kappa\|_{L^2_r L^\infty_c}^{2\beta-1} \|J\kappa\|_{L^4_x L^2_y}^2.\tag{7.19}$$

The term on the right-hand side of (7.18) is of the same form obtained in (7.15), while the term (7.19) can be estimated using (3.17) followed by the usual (3.14):

$$\begin{aligned}\|dg_2(\rho_\gamma)\rho_{J^s\gamma}\,\kappa\|_{W^0} &\lesssim \|\kappa\|_{L^2_r L^\infty_c}^{2\beta} \|J^s\kappa\|_{W^0} + \|\kappa\|_{L^2_r L^\infty_c}^{2\beta-1} \|J\kappa\|_{L^2_r L^4_c}^2\\ &\lesssim t^{-d\beta} \|\kappa\|_{W^2}^{2\beta} \|J^s\kappa\|_{W^0} + t^{-d/2} \|\kappa\|_{L^2_r L^\infty_c}^{2\beta-1} \|J^2\kappa\|_{W^0}^{d/2} \|J\kappa\|_{W^0}^{(4-d)/2}\\ &\lesssim t^{-d\beta} \|\kappa\|_{W^2}^{2\beta+1} \end{aligned}$$

having used $\beta \ge 1/2$ in the last inequality.

Now, we consider (7.7) for $i = 2$ with $k = 1$ and $|s| = 1 = |a|$. We compute as in (7.14)

$$\begin{aligned} \|dg_2(\rho_\gamma)(\rho_{J\gamma})\, J\kappa\|_{W^0}^2 &= \beta^2 \int_{\mathbb{R}^3} \rho_\gamma^{2\beta-2}(x)\, \rho_{J\gamma}^2(x)\, (\int_{\mathbb{R}^3} |J\kappa(x,y)|^2 dy) dx \\ &= \beta^2 \int_{\mathbb{R}^3} \rho_\gamma^{2\beta-2}(x)\, \rho_{J\gamma}^2(x) \rho_{J\kappa^* J\kappa}(x)\, dx. \end{aligned} \tag{7.20}$$

Using the inequality (5.6), we find

$$\begin{aligned} \|dg_2(\rho_\gamma)(\rho_{J\gamma})\, J\kappa\|_{W^0}^2 &\le 2\beta^2 \int_{\mathbb{R}^3} \rho_\gamma^{2\beta-1}(x)\, \rho_{J\kappa^* J\kappa}(x) \rho_{J\kappa^* J\kappa}(x)\, dx \\ &\lesssim \beta^2 \|\kappa\|_{L_r^2 L_c^\infty}^{4\beta-2} \|J\kappa\|_{L_x^4 L_y^2}^4. \end{aligned}$$

The right-hand side is a product of terms we treated above and we see that

$$\|dg_2(\rho_\gamma)(\rho_{J\gamma})\, J\kappa\|_{W^0} \lesssim t^{-d\beta} \|\kappa\|_{W^2}^{2\beta+1}. \tag{7.21}$$

Finally, we consider (7.7) for $i = 2$ with $k > 1, a = 0$ and $|s| = 1$. We compute as in (7.14)

$$\begin{aligned} \|d^k g_2(\rho_\gamma)(\rho_{J\gamma})^k\, \kappa\|_{W^0}^2 &= (\beta(1-\beta))^2 \int_{\mathbb{R}^3} \rho_\gamma^{2\beta-2k}(x)\, \rho_{J\gamma}^{2k}(x)\, (\int_{\mathbb{R}^3} |\kappa(x,y)|^2 dy) dx \\ &= (\beta(1-\beta))^2 \int_{\mathbb{R}^3} \rho_\gamma^{2\beta-2k+1}(x)\, \rho_{J\gamma}^{2k}(x)\, dx. \end{aligned} \tag{7.22}$$

Using (5.6) in (7.22), we find, for $\beta \ge (k-1)/2$,

$$\begin{aligned} \|d^k g_2(\rho_\gamma)(\rho_{J\gamma})^k\, \kappa\|_{W^0}^2 &\lesssim \int_{\mathbb{R}^3} \rho_\gamma^{2\beta-k+1}(x)\, \rho_{J\kappa^* J\kappa}^k(x)\, dx \\ &\lesssim \|\kappa\|_{L_r^2 L_c^\infty}^{4\beta-2k+2} \|J\kappa\|_{L_x^4 L_y^2}^{2k}. \end{aligned}$$

The square root of this last quantity is again a product of terms like those treated above and, using (3.17) and (3.14), can be bound by the right-hand side of (7.21). This concludes the proof of (7.7)-(7.8) and the energy estimate (7.1). $\square$

Remark 7.2 (Higher dimensions). The calculation done for general $k > 1$ in (7.22) shows that one can close this type of estimates even for $k > 2$ provided $\beta \ge (k-1)/2$. Since we need $k = [d/2] + 1$ derivatives to deduce the necessary sharp $L_c^\infty L_r^2$ decay (through (3.14)), this means that in dimension $d > 3$ it is possible to treat the case of $\mathrm{xc}(\rho) = \rho^\beta$ for $\beta \ge (1/2)[d/2]$. Of course, when applying k derivatives with $k > 2$ there are several other terms to consider besides (7.22); however, these other terms can all be treated with similar arguments to those in the proof of Lemma 7.1 above, using (3.17) and proper applications of (3.14).

8. Local existence, GWP and scattering for (3.1)

In this section we will use the non-abelian analogues of Sobolev spaces based on the space of Hilbert-Schmidt operators introduced in (4.1), which we recall here for convenience:

$$V^s := \big\{\kappa \in I^2 \,:\, \sum_{|\alpha|\le s} \|D^\alpha \kappa\|_{I^2} < \infty\big\}, \tag{8.1}$$

with $D_\ell \kappa := [\partial_{x_\ell}, \kappa], D = (D_1, \dots, D_d) = [\nabla, \cdot]$, for any positive integer s. Note that $V^0 = I^2 = W^0$, see (1.7) and (1.11).

Theorem 8.1 (Local existence)**.** *Assume* (1.13)-(1.20) *and consider equation* (3.1) *with initial data $\kappa(0) = \kappa_0$. Then we have the following:*

(i) *(Local existence) If $\kappa_0 \in V^{[d/2]+1}$, then there exists $T_0 = T_0(\|\kappa_0\|_{V^{[d/2]+1}}) > 0$ and a unique solution $\kappa \in C([-T_0, T_0], V^{[d/2]+1})$ of* (3.1) *with $\kappa(0) = \kappa_0$.*

(ii) *(Energy Estimate) If $\kappa_0 \in V^k$, $k \ge [d/2]+1$, then the solution $\kappa \in C([-T_0, T_0], V^{[d/2]+1})$ of* (3.1) *from part (i) satisfies the following energy estimate:*

$$\frac{d}{dt}\|\kappa(t)\|_{V^k} \le \lambda |t|^{-p} \cdot P(\|\kappa(t)\|_{W^{[d/2]+1}}) \cdot \|\kappa(t)\|_{V^k} \tag{8.2}$$

for some $p > 1$ (depending on g), where $\lambda = |\lambda_1| + |\lambda_2|$, and P is a polynomial with positive coefficients which depend on g,d and k.

(iii) *(Continuity of the weighted norm) For $\kappa_0 \in V^k \cap W^b$, with $[d/2] + 1 \le b \le k$, the map $t \to \kappa(t)$ is continuous from $[-T_0, T_0]$ to $V^k \cap W^b$.*

Proof. (i) Denote by α_t the linear flow associated with the operator $\kappa \mapsto i[-\Delta, \kappa]$. Note that α_t is unitary on V^k. We obtain the solution κ as a fixed point of the map

$$\Phi(\kappa(t)) = \alpha_t(\kappa_0) + \int_0^t \alpha_{t-s}\big(\big[g(\rho(\gamma(s))), \kappa(s)\big]\big) ds \tag{8.3}$$

in the space

$$\big\{\kappa \in C([-T_0, T_0], V^{[d/2]+1}), \sup_{[-T_0,T_0]} \|\kappa(t)\|_{V^{[d/2]+1}} \le 2\|\kappa_0\|_{V^{[d/2]+1}}\big\},$$

for a sufficiently small T_0. For this it suffices to prove, for all $k \le [d/2]+1$, the estimates

$$\|\Phi(\kappa(t))\|_{V^{[d/2]+1}} \le \|\kappa_0\|_{V^{[d/2]+1}} + \int_0^t P\big(\|\kappa(s)\|_{V^{[d/2]+1}}\big) ds, \tag{8.4}$$

$$\|\Phi(\kappa_1(t)) - \Phi(\kappa_2(t))\|_{V^{[d/2]+1}} \le \int_0^t Q\big(\|\kappa\|_{V^{[d/2]+1}}\big) \|\kappa_1(s) - \kappa_2(s)\|_{V^{[d/2]+1}} ds, \tag{8.5}$$

for some polynomials P and Q with positive coefficients.

To prove (8.4) we first notice that $[D, \alpha_t] = 0$ and thus (8.4) can be reduced to proving that for all $k \le [d/2] + 1$

$$\|D^k\big[g(\rho(\gamma)), \kappa\big]\|_{V^0} \lesssim P\big(\|\kappa\|_{V^{[d/2]+1}}\big). \tag{8.6}$$

Estimate (8.6) then follows similarly to the proof of Proposition 7.1, (which deals with J and the space W^k instead of D and the space V^k). First we commute D with the vector-field $D_\gamma\kappa := \partial_t\kappa - i[h_\gamma, \kappa]$ (in the same way that we commuted J in Proposition 6.2) to obtain

$$D_\gamma D\kappa = DD_\gamma\kappa + i[dg(\rho_\gamma)\rho_{D\gamma}, \kappa] \tag{8.7}$$

We then use $\|f\kappa\|_{V^0} \lesssim \|f\|_{L^p}\|\kappa\|_{L^2_rL^s_c}$, $1/p + 1/s = 1/2$, see (5.4), and (5.1), followed by the Gagliardo-Nirenberg-Sobolev type inequality

$$\|\kappa\|_{L^2_rL^s_c} \lesssim \|\kappa\|^{\alpha}_{V^b}\|\kappa\|^{1-\alpha}_{V^0}, \tag{8.8}$$

for $\alpha b = d(\frac{1}{2} - \frac{1}{s})$, $s \geq 2$, see (4.9), to find (8.4). The proof of the estimate for the differences is similar so we skip the details.

(ii) In Lemma 7.1 we proved a more precise version of (8.2) with the weighted W^k-norm replacing the V^k-norm. Therefore, we leave to the reader the details of the proof of the more standard energy inequality (8.2) which follows from similar arguments.

(iii) This property follows from similar (short-time) energy estimates. Continuity of the map $t \in [0, T] \mapsto \kappa(t) \in V^k$ follows essentially from (8.6) which also shows

$$\frac{d}{dt}\|\kappa(t)\|_{V^k} \lesssim P\big(\|\kappa\|_{V^{[d/2]+1}}\big).$$

Continuity in the weighted space, W^b, follows from the analogous weighted energy estimate

$$\frac{d}{dt}\|\kappa(t)\|_{W^k} \lesssim P\big(\|\kappa\|_{V^{[d/2]+1}}\big)\|\kappa(t)\|_{W^k}, \tag{8.9}$$

which can be obtained by the exact same arguments used in the proof of (7.1), making use of (8.8) instead of (3.14). □

Proof of Proposition 3.5. In view of item (i) of Theorem 8.1, in order to continue a local-in-time solution of (3.1) to a global one, it suffices to obtain a uniform in time a priori bound for the V^k-norm with $k \geq [d/2] + 1$. This follows by an application of Gronwall's inequality to (8.2) with the uniform bound $\|\kappa(t)\|_{W^{[d/2]+1}} \lesssim \|\kappa_0\|_{W^{[d/2]+1}}$ given by (3.16) in Proposition 3.8.

The scattering property for equation (3.1) in the space V^0 (also in $V^k \cap W^b$, $[d/2]+1 \leq b \leq k$) is proven by standard arguments as follows. Let $\alpha_t(\kappa)$ be the linear evolution $\alpha_t(\kappa) := e^{i\Delta t}\kappa e^{-i\Delta t}$. Define $\tilde\kappa(t) := \alpha_{-t}(\kappa(t))$ and use (3.1) to compute

$$\partial_t\tilde\kappa(t) = \alpha_{-t}(i[g(\rho_{\kappa^*\kappa}), \kappa(t)]).$$

Writing $\tilde\kappa(t)$ as the integral of its derivative, using the above relation, taking the ($I^2 = V^0$)-norm of the resulting identity and using the unitarity of α_{-r} gives

$$\begin{aligned}\|\tilde\kappa(t) - \tilde\kappa(s)\|_{V^0} &\lesssim \int_s^t \|\alpha_{-\tau}(i[g(\rho_{\kappa^*\kappa}), \kappa(\tau)])\|_{V^0}\, d\tau \\ &\lesssim \int_s^t \|[g(\rho_{\kappa^*\kappa}), \kappa(\tau)]\|_{V^0}\, d\tau. \end{aligned} \tag{8.10}$$

Then we apply estimate (5.4) with $p = \infty, s = 2$, use the conditions (1.14) and (1.19) on g_1 and g_2, the estimate (5.3) (with $b = b' = [d/2] + 1$, so that in particular $\alpha, \alpha' < 1$), to obtain

$$\begin{aligned}\|[g(\rho_{\kappa^*\kappa}),\kappa(\tau)]\|_{V^0} &\lesssim \|g(\rho_{\kappa^*\kappa})\|_\infty \|\kappa(\tau)\|_{V^0}\\ &\lesssim \left(\|\rho_{\kappa^*\kappa}\|_q^a + \|\rho_{\kappa^*\kappa}\|_\infty^\beta\right)\|\kappa(\tau)\|_{V^0}\\ &\lesssim \left(|\tau|^{-d(1-1/q)a} + |\tau|^{-d\beta}\right)\|\kappa(\tau)\|^2_{W^{[d/2]+1}}\|\kappa(\tau)\|_{V^0}, \end{aligned} \tag{8.11}$$

where the parameters a and β above are those appearing in (1.14) and (1.21). Since a and β satisfy $d(1-1/q)a$ and $d\beta > 1$, the integrand in (8.10) is integrable in time. Hence $\tilde{\kappa}(t)$ has the Cauchy property and therefore converges to some $\kappa_\infty \in V^0$ as $t \to \infty$. This implies

$$\|\kappa(t) - e^{i\Delta t}\kappa_\infty e^{-i\Delta t}\|_{V^0} \to 0. \tag{8.12}$$

□

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