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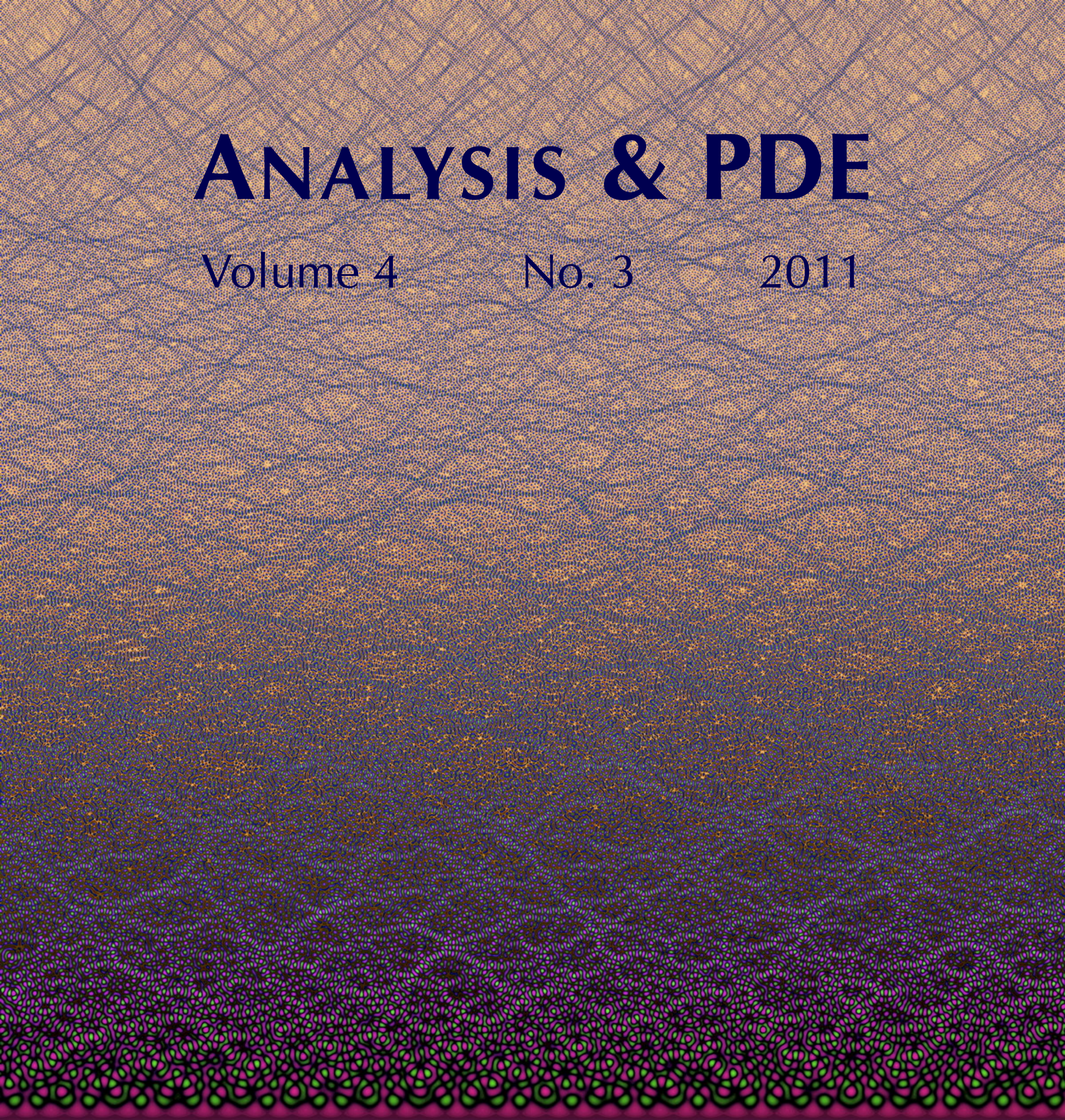

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REGULARITY OF WEAK SOLUTIONS OF A COMPLEX MONGE–AMPÈRE EQUATION

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We prove the smoothness of weak solutions to an elliptic complex Monge–Ampère equation, using the smoothing property of the corresponding parabolic flow.

1. Introduction

Let (M, ω) be a compact Kähler manifold. Our main result is the following.

Theorem 1. *Suppose that $\varphi \in PSH(M, \omega) \cap L^\infty(M)$ is a solution of the equation*

$$(\omega + \sqrt{-1}\partial\overline{\partial}\varphi)^n = e^{-F(\varphi,z)}\omega^n$$

in the sense of pluripotential theory [Bedford and Taylor 1976], where $F : \mathbb{R} \times M \to \mathbb{R}$ is smooth. Then φ is smooth.

In particular, if M is Fano, $\omega \in c_1(M)$, and h_ω satisfies $\sqrt{-1}\partial\overline{\partial}h_\omega = \mathrm{Ric}(\omega) - \omega$, then we can set $F(\varphi, z) = \varphi - h_\omega$. The result then implies that Kähler–Einstein currents with bounded potentials are in fact smooth. Such weak Kähler–Einstein metrics were studied by Berman, Boucksom, Guedj, and Zeriahi in [Berman et al. 2009], as part of their variational approach to complex Monge–Ampère equations.

It follows from [Kołodziej 2008] (see also [Guedj et al. 2008]) that the solution φ in Theorem 1 is automatically C^α for some $\alpha > 0$, but it does not seem possible to use this directly to get further regularity. The difficulty is that in the equation

$$(\omega + \sqrt{-1}\partial\overline{\partial}\varphi)^n = e^f\omega^n,$$

the C^1 estimate for φ (due to Błocki [2009] and Hanani [1996]) depends on a C^1 bound for f, and in turn the Laplacian estimate for φ (due to Yau [1978] and Aubin [1976]) depends on the Laplacian of f.

To get around this difficulty we look at the corresponding parabolic flow

$$\frac{\partial\varphi}{\partial t} = \log\frac{(\omega + \sqrt{-1}\partial\overline{\partial}\varphi)^n}{\omega^n} + F(\varphi, z).$$

Following the construction of [Song and Tian 2009] for the Kähler–Ricci flow, we show that to find a solution for a short time, it is enough to have a C^0 initial condition φ_0 for which $(\omega + \sqrt{-1}\partial\overline{\partial}\varphi_0)^n$ is bounded (see also [Chen and Ding 2007; Chen and Tian 2008; Chen et al. 2011] for earlier results, as well as [Simon 2002] for a weaker statement in the Riemannian case). The solution of the flow will be smooth at any positive time. Then we need to argue that if the initial condition φ_0 is a weak solution of the elliptic problem then the flow is stationary, so in fact φ_0 is smooth.

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In Section 2 we show that the flow (with smooth initial data) exists for a short time, which only depends on a bound for $\sup|\varphi_0|$ and $\sup|\dot{\varphi}_0|$. In Section 3 we use this to construct a solution to the flow with rough initial data, and we prove Theorem 1.

2. Existence for the parabolic equation

In this section we consider the parabolic equation

$$\frac{\partial\varphi}{\partial t} = \log\frac{(\omega+\sqrt{-1}\partial\bar{\partial}\varphi)^n}{\omega^n} + F(\varphi, z), \tag{1}$$

where $F : \mathbb{R}\times M \to \mathbb{R}$ is smooth and we have the smooth initial condition $\varphi|_{t=0} = \varphi_0$. We write $\dot{\varphi}_0$ for $\partial\varphi/\partial t$ at $t = 0$.

The main result of this section is the following:

Proposition 2. *There exist $T > 0$ depending only on* $\sup|\varphi_0|$, $\sup|\dot{\varphi}_0|$ (*and ω and F*), *such that there is a smooth solution $\varphi(t, z) : [0, T]\times M \to \mathbb{R}$ to* (1). *We also have smooth functions $C_k : (0, T] \to \mathbb{R}$ depending only on* $\sup|\varphi_0|$, $\sup|\dot{\varphi}_0|$ *such that*

$$\|\varphi(t)\|_{C^k(M)} < C_k(t) \tag{2}$$

as long as $t \leqslant T$. (Note that $C_k(t) \to \infty$ as $t \to 0$.)

The proof of the C^1 estimate is based on the arguments in [Błocki 2009] (see also [Hanani 1996; Phong and Sturm 2010]), whereas the C^2 estimate is based on the Aubin–Yau second order estimate [Aubin 1976; Yau 1978] (see also [Song and Tian 2009] for the parabolic version we need here). The C^3 and higher order estimates follow the standard arguments in [Yau 1978; Cao 1985; Phong et al. 2007], although there are a few new terms to control.

The existence of a smooth solution for $t \in [0, T')$ for some $T' > 0$ that depends on the $C^{2,\alpha}$ norm of φ_0 is standard. The aim is to obtain the estimates (2), which allow us to extend the solution up to a time T, which only depends on the initial condition in a weaker way. We will write $\varphi(t)$ for the short time solution.

Lemma 3. *There exists $T, C > 0$ depending only on* $\sup|\varphi_0|$ *and* $\sup|\dot{\varphi}_0|$ *such that*

$$|\varphi(t)|, |\dot{\varphi}(t)| < C, \tag{3}$$

as long as the solution exists and $t \leqslant T$. In particular,

$$\left|\log\frac{(\omega+\sqrt{-1}\partial\bar{\partial}\varphi)^n}{\omega^n}\right| < C \tag{4}$$

for $t \leqslant T$.

Proof. For all s, define

$$\bar{F}(s) = \sup\nolimits_{z\in M} F(s, z),$$

which is a continuous function. At any given time t where φ exists, the maximum of $\varphi(t,\cdot)$ is achieved at some point $z \in M$, and at z we have

$$\log\frac{(\omega+\sqrt{-1}\partial\bar{\partial}\varphi)^n}{\omega^n} \leqslant 0.$$

It follows that
$$\frac{d\varphi_{\max}}{dt} \leqslant F(\varphi_{\max}, z) \leqslant \bar{F}(\varphi_{\max}),$$
where the derivative is interpreted as the limsup of the forward difference quotients at the points where it does not exist (compare [Hamilton 1986, Lemma 3.5]). Comparing with the solution of the corresponding ODE, we find that there exist $T, C > 0$ depending only on $\sup|\varphi_0|$ such that as long as our solution exists, and $t \leqslant T$, we have $\sup \varphi(t) < C$. In a similar way we get a lower bound on $\varphi(t, \cdot)$, so we have $|\varphi(t)| < C$ as long as the solution exists and $t \leqslant T$.

Differentiating the equation we obtain
$$\frac{\partial \dot{\varphi}}{\partial t} = \Delta_\varphi \dot{\varphi} + F'(\varphi, z)\dot{\varphi}, \tag{5}$$
where F' is the derivative of F with respect to the φ variable. Since $F'(\varphi, z)$ is bounded as long as φ is bounded, from the maximum principle we get
$$\sup|\dot{\varphi}(t)| < \sup|\dot{\varphi}(0)|e^{\kappa t}, \tag{6}$$
where κ depends on F and $\sup|\varphi(0)|$. Hence for our choice of T, we get
$$\sup|\dot{\varphi}(t)| < C,$$
for $t \leqslant T$, where C depends on $\sup|\varphi_0|$ and $\sup|\dot{\varphi}_0|$. □

In the lemmas below T will be the same as in the previous lemma.

Lemma 4. *There exists $C > 0$ depending on $\sup|\varphi_0|$ and $\sup|\dot{\varphi}_0|$ such that*
$$|\nabla\varphi(t)|^2_\omega < e^{C/t}, \tag{7}$$
as long as the solution exists and $t \leqslant T$ for the T in Lemma 3.

Proof. We modify Błocki's estimate [2009] for the complex Monge–Ampère equation (compare [Hanani 1996]). Define
$$K = t\log|\nabla\varphi|^2_\omega - \gamma(\varphi),$$
where γ will be chosen later. Suppose that $\sup_{(0,t]\times M} K = K(t, z)$ is achieved. Pick normal coordinates for ω at z, such that $\varphi_{i\bar{j}}$ is diagonal at this point (here and henceforth, indices will denote covariant derivatives with respect to the metric ω). We write $\beta = |\nabla\varphi|^2_\omega$ and Δ_φ for the Laplacian of the metric $\omega + \sqrt{-1}\partial\bar{\partial}\varphi$. There exists $B > 0$ such that
$$\begin{aligned} 0 \leqslant \Big(\frac{\partial}{\partial t} - \Delta_\varphi\Big)K \leqslant -\frac{t}{\beta}\sum_{i,p}\frac{|\varphi_{ip}|^2 + |\varphi_{i\bar{p}}|^2}{1+\varphi_{p\bar{p}}} + (t^{-1}(\gamma')^2 + \gamma'')\sum_p \frac{|\varphi_p|^2}{1+\varphi_{p\bar{p}}} \\ -(\gamma' - Bt)\sum_p \frac{1}{1+\varphi_{p\bar{p}}} + \log\beta + \frac{Ct}{\beta} - \gamma'\dot{\varphi} + n\gamma' + Ct. \end{aligned}$$
The constant C depends on bounds for F and F', and also we used that $\nabla K = 0$ at (t, z).

Now we apply Błocki's trick to get rid of the term containing $(\gamma')^2$. At (t, z) we have
$$t\beta_p = \gamma'\beta\varphi_p,$$

where

$$\beta_p = \varphi_p \varphi_{p\bar{p}} + \sum_j \varphi_{jp} \varphi_{\bar{j}},$$

remembering that $\varphi_{j\bar{p}}$ is diagonal. It follows that

$$\sum_j \varphi_{jp} \varphi_{\bar{j}} = (t^{-1}\gamma'\beta - \varphi_{p\bar{p}})\varphi_p,$$

and so

$$\frac{t}{\beta}\sum_{j,p}\frac{|\varphi_{jp}|^2}{1+\varphi_{p\bar{p}}} \geqslant \frac{t}{\beta^2}\sum_p \frac{\left|\sum_j \varphi_{jp}\varphi_{\bar{j}}\right|^2}{1+\varphi_{p\bar{p}}} = \frac{t}{\beta^2}\sum_p \frac{|t^{-1}\gamma'\beta - \varphi_{p\bar{p}}|^2|\varphi_p|^2}{1+\varphi_{p\bar{p}}} \geqslant t^{-1}(\gamma')^2\sum_p \frac{|\varphi_p|^2}{1+\varphi_{p\bar{p}}} - 2\gamma',$$

where we assume that $\gamma' > 0$. Also from Lemma 3 we know that $\dot{\varphi}$ is bounded. Combining these estimates we obtain

$$0 \leqslant \gamma''\sum_p \frac{|\varphi_p|^2}{1+\varphi_{p\bar{p}}} - (\gamma' - Bt)\sum_p \frac{1}{1+\varphi_{p\bar{p}}} + \log\beta + \frac{Ct}{\beta} + C\gamma' + Ct.$$

We now choose $\gamma(s) = As - \frac{1}{A}s^2$. We can assume that $\log\beta > 1$ at (t, z), so in particular $\frac{t}{\beta}$ is bounded above as long as $t < T$. Then if A is chosen sufficiently large, we get a constant $C' > 0$ such that

$$\sum_p \frac{1}{1+\varphi_{p\bar{p}}} + \sum_p \frac{|\varphi_p|^2}{1+\varphi_{p\bar{p}}} \leqslant C'\log\beta, \tag{8}$$

so in particular $(1+\varphi_{p\bar{p}})^{-1} \leqslant C'\log\beta$ for each p. From (4) we know that

$$\prod_p (1+\varphi_{p\bar{p}}) < C,$$

so

$$1+\varphi_{p\bar{p}} \leqslant C(C'\log\beta)^{n-1},$$

and using (8) we get

$$\beta = \sum_p |\varphi_p|^2 \leqslant C(C'\log\beta)^n.$$

This shows that $\beta < C$ and in turn $K < C$ for some constant C. So either K achieves a maximum for some $t > 0$ in which case we have just bounded it, or it achieves its maximum for $t = 0$, which is bounded in terms of $\sup|\varphi_0|$. □

From now on, we write g for the metric ω and g_φ for the metric $\omega + \sqrt{-1}\partial\bar{\partial}\varphi$.

Lemma 5. *There exists $C > 0$ depending on* $\sup|\varphi_0|$ *and* $\sup|\dot{\varphi}_0|$ *such that*

$$0 < \mathrm{tr}_g(g_\varphi) = n + \Delta_g\varphi(t) < e^{Ce^{C/t}}, \tag{9}$$

as long as the solution exists and $t \leqslant T$, where T is as in Lemma 3.

Proof. We let

$$H = e^{-\alpha/t}\log\mathrm{tr}_g(g_\varphi) - A\varphi,$$

where $\alpha = C$ from Lemma 4 and A is chosen later. In particular we will use that $e^{-\alpha/t}|\nabla\varphi|_g^2 < 1$. Standard calculations (from [Aubin 1976; Yau 1978]) show that there exist $B > 0$ such that

$$\Delta_\varphi \log \operatorname{tr}_g(g_\varphi) \geqslant -B \operatorname{tr}_{g_\varphi} g - \frac{\operatorname{tr}_g \operatorname{Ric}(g_\varphi)}{\operatorname{tr}_g(g_\varphi)}.$$

Using this we can compute

$$\begin{aligned}\Big(\frac{\partial}{\partial t} - \Delta_\varphi\Big)H \\ \leqslant \frac{\alpha e^{-\alpha/t}}{t^2} \log \operatorname{tr}_g(g_\varphi) + \frac{Ce^{-\alpha/t}}{\operatorname{tr}_g(g_\varphi)} + \frac{e^{-\alpha/t}\Delta_g F(\varphi, z)}{\operatorname{tr}_g(g_\varphi)} + Be^{-\alpha/t} \operatorname{tr}_{g_\varphi} g - A\dot\varphi + An - A \operatorname{tr}_{g_\varphi} g. \quad (10)\end{aligned}$$

Here

$$\Delta_g F(\varphi, z) = \Delta_g F + 2\operatorname{Re}(g^{i\bar j} F_i' \varphi_{\bar j}) + F'\Delta_g\varphi + F''|\nabla\varphi|_g^2,$$

where F' is the derivative in the φ variable, and $\Delta_g F$ is the Laplacian of $F(\varphi, z)$ in the z variable. So we have constants C_1, C_2, C_3 such that

$$\Delta_g F(\varphi, z) \leqslant C_1 + C_2|\nabla\varphi|_g^2 + C_3 \operatorname{tr}_g(g_\varphi).$$

From (4) we have bounds on above and below on $\frac{\det g_\varphi}{\det g}$, so for some constant C we have $\operatorname{tr}_g(g_\varphi) > C^{-1}$ and also $\operatorname{tr}_g(g_\varphi) \leqslant C(\operatorname{tr}_{g_\varphi} g)^{n-1}$. Using these in (10) we get

$$\begin{aligned}\Big(\frac{\partial}{\partial t} - \Delta_\varphi\Big)H &\leqslant -(A - Be^{-\alpha/t}) \operatorname{tr}_{g_\varphi} g + C \log \operatorname{tr}_{g_\varphi} g + C \\ &\leqslant -(A - C - Be^{-\alpha/t}) \operatorname{tr}_{g_\varphi} g + C',\end{aligned}$$

as long as $t \leqslant T$. Choosing A large enough, we can use the maximum principle to bound H in terms of its value for $t = 0$, which is bounded by $\sup|\varphi_0|$. □

We note here that if one is interested in the special case of weak Kähler–Einstein currents (i.e., $F = \varphi - h_\omega$), then the gradient estimate in Lemma 4 is not needed. We now describe how to get the higher order estimates, as long as the solution exists and $t \leqslant T$, for the T from Lemma 3. As in [Yau 1978], we let $\varphi_{i\bar j k}$ be the third covariant derivative of φ with respect to the Levi-Civita connection of ω, and we define

$$S = g_\varphi^{i\bar p} g_\varphi^{q\bar j} g_\varphi^{k\bar r} \varphi_{i\bar j k} \varphi_{\bar p q \bar r}.$$

From now on, we will denote by $C(t)$ a smooth real function defined on $(0, T]$, which is allowed to blow up when t approaches zero, which depends only on $\sup|\varphi_0|$, $\sup|\dot\varphi_0|$ and which may vary from line to line. These functions $C(t)$ can be made completely explicit. Using (9) it is clear that an estimate of the form $S \leqslant C(t)$ implies an estimate of the form $\|\varphi(t)\|_{C^{2+\alpha}(g)} \leqslant C(t)$, for any $0 < \alpha < 1$. To estimate S we first compute its evolution. It is convenient to use the general computation by Phong, Šešum, and Sturm [Phong et al. 2007], which uses the following notation. We denote by $h^i_j = g^{i\bar k}(g_{j\bar k} + \varphi_{j\bar k})$, which is an endomorphism of the tangent bundle. Then S can be written in terms of the connection ∇hh^{-1} as

$$S = g_\varphi^{p\bar q} g_{\varphi, i\bar j} g_\varphi^{k\bar\ell} (\nabla_p hh^{-1})^i_k \overline{(\nabla_q hh^{-1})^j_\ell} = |\nabla hh^{-1}|^2_{g_\varphi},$$

where ∇ is the Levi-Civita connection of ω_φ. Then the computations in [Phong et al. 2007] yield

$$\Big(\frac{\partial}{\partial t}-\Delta_\varphi\Big)S=-|\nabla(\nabla hh^{-1})|^2_{g_\varphi}-|\overline{\nabla}(\nabla hh^{-1})|^2_{g_\varphi}+2\,\mathrm{Re}\big\langle(\nabla T-\nabla R,\,\nabla hh^{-1}\big\rangle_{g_\varphi}$$
$$+(\nabla_p hh^{-1})^i_k\overline{(\nabla_q hh^{-1})^j_\ell}(T^{p\bar q}g_{\varphi,i\bar j}g_\varphi^{k\bar\ell}-g_\varphi^{p\bar q}T_{i\bar j}g_\varphi^{k\bar\ell}+g_\varphi^{p\bar q}g_{\varphi,i\bar j}T^{k\bar\ell}),$$

where $T_{i\bar j}=-\big(\partial g_\varphi/\partial t+\mathrm{Ric}(g_\varphi)\big)_{i\bar j}$, $(\nabla T)^p_{qr}=g_\varphi^{p\bar s}\nabla_q T_{r\bar s}$, $(\nabla R)^p_{qr}=g_\varphi^{s\bar t}\nabla_s R^p_{rq\bar t}$ and $R^p_{rq\bar t}$ is the curvature of the fixed metric g. Along the standard Kähler–Ricci flow the tensor T vanishes, while in our case differentiating (1) we get

$$-T_{i\bar j}=\mathrm{Ric}(g)_{i\bar j}+F''\varphi_i\varphi_{\bar j}+F'\varphi_{i\bar j}+F_{i\bar j}+2\,\mathrm{Re}(F_i'\varphi_{\bar j}). \tag{11}$$

Using (7) and (9) we can then estimate

$$\big|(\nabla_p hh^{-1})^i_k\overline{(\nabla_q hh^{-1})^j_\ell}(T^{p\bar q}g_{\varphi,i\bar j}g_\varphi^{k\bar\ell}-g_\varphi^{p\bar q}T_{i\bar j}g_\varphi^{k\bar\ell}+g_\varphi^{p\bar q}g_{\varphi,i\bar j}T^{k\bar\ell})\big|\leqslant C(t)S.$$

The term $2\,\mathrm{Re}\langle\nabla R,\,\nabla hh^{-1}\rangle_{g_\varphi}$ is comparable to S, but bounding $2\,\mathrm{Re}\langle\nabla T,\,\nabla hh^{-1}\rangle_{g_\varphi}$ requires a bit more work. Differentiating (11) and using (3), (7) and (9) we see that all the terms in $2\,\mathrm{Re}\langle\nabla T,\,\nabla hh^{-1}\rangle_{g_\varphi}$ are comparable to $C(t)S$ except for two terms of the form

$$\langle\varphi_{ij}g_\varphi^{k\bar\ell}\varphi_{\bar\ell},\,(\nabla_i hh^{-1})^k_j\rangle_{g_\varphi}.$$

We bound these by $|\varphi_{ij}|^2_{g_\varphi}+C(t)S$, so overall we get

$$\Big(\frac{\partial}{\partial t}-\Delta_\varphi\Big)S\leqslant C(t)S+|\varphi_{ij}|^2_{g_\varphi}+C.$$

The term $C(t)S$ can be controlled by using $\mathrm{tr}_g(g_\varphi)$ in the usual way [Phong et al. 2007]. For the term $|\varphi_{ij}|^2_{g_\varphi}$ we note that using (3), (7) and (9) we have

$$\Big(\frac{\partial}{\partial t}-\Delta_\varphi\Big)|\nabla\varphi|^2_g\leqslant-\sum_{i,p}\frac{|\varphi_{ip}|^2+|\varphi_{i\bar p}|^2}{1+\varphi_{p\bar p}}+2\,\mathrm{Re}\langle\nabla\varphi,\,F'\nabla\varphi+\nabla F\rangle_g+C\,\mathrm{tr}_{g_\varphi}g|\nabla\varphi|^2_g$$
$$\leqslant-\frac{|\varphi_{ij}|^2_{g_\varphi}}{C(t)}+C(t).$$

We can then apply the maximum principle to the quantity

$$G=\frac{S}{C_1(t)}+\frac{\mathrm{tr}_g(g_\varphi)}{C_2(t)}+\frac{|\nabla\varphi|^2_g}{C_3(t)},$$

for suitable functions $C_i(t)$ that depend only on the given data, and get $G\leqslant C$, which implies the desired estimate for S. This means that as long as the solution exists and $0<t\leqslant T$ we have a bound on $\|\varphi(t)\|_{C^{2+\alpha}(M)}$. Since by standard parabolic theory one can start the flow with initial data in $C^{2+\alpha}$, this shows that the flow has a $C^{2+\alpha}$ solution defined on $[0,T]$.

The next step is to estimate $\sup|\ddot\varphi(t)|$ and $\sup|\partial_i\partial_{\bar j}\dot\varphi(t)|$. It is easy to see that both of these quantities are bounded if we bound $|\mathrm{Ric}(g_\varphi)|_{g_\varphi}$. Following the computation in [Phong et al. 2011, p. 107] one can derive the following estimate (there are essentially no new bad terms in this case)

$$\Big(\frac{\partial}{\partial t}-\Delta_\varphi\Big)|\mathrm{Ric}(g_\varphi)|_{g_\varphi}\leqslant C(t)|\mathrm{Rm}(g_\varphi)|^2+C(t).$$

From one of the two good positive terms in the evolution of S we get

$$\Big(\frac{\partial}{\partial t}-\Delta_\varphi\Big)S \leqslant -\frac{|\mathrm{Rm}(g_\varphi)|^2}{C(t)}+C(t)$$

and so the maximum principle applied to the quantity

$$\frac{|\mathrm{Ric}(g_\varphi)|_{g_\varphi}}{C_1(t)}+\frac{S}{C_2(t)}$$

gives the desired bound $|\mathrm{Ric}(g_\varphi)|_{g_\varphi} \leqslant C(t)$.

It now follows from the parabolic Schauder estimates applied to (5) that we have bounds for φ in the parabolic Hölder space $C^{2+\alpha,1+\alpha/2}(M\times[\varepsilon,T])$ for any $\varepsilon>0$, with the bounds only depending on ε, $\sup|\varphi_0|$ and $\sup|\dot{\varphi}_0|$. By the parabolic Schauder estimates we then also get bounds on all higher order derivatives for φ, and letting $\varepsilon\to 0$ we get the required bounds on $\varphi(t)$ that blow up as t goes to zero. In particular, we get a smooth solution $\varphi(t)$ that exists on $[0, T]$, with bounds as in (2). This completes the proof of Proposition 2.

3. Proof of Theorem 1

Suppose that φ is a bounded ω-plurisubharmonic solution of the equation

$$(\omega+\sqrt{-1}\partial\overline{\partial}\varphi)^n = e^{-F(\varphi,z)}\omega^n, \tag{12}$$

where F is a smooth function. First of all we want to prove existence of the flow (1) with rough initial data φ. For this, we follow the proof in [Song and Tian 2009] in the case of Kähler–Ricci flow.

It follows from [Kołodziej 1998] that in this case φ is continuous (in fact it is even C^α; see [Guedj et al. 2008; Kołodziej 2008]). Let us approximate φ with a sequence of smooth functions u_k, such that

$$\sup_M |\varphi-u_k| \to 0, \tag{13}$$

as $k\to\infty$. By the theorem in [Yau 1978] there are smooth functions ψ_k such that

$$(\omega+\sqrt{-1}\partial\overline{\partial}\psi_k)^n = c_k e^{-F(u_k,z)}\omega^n, \tag{14}$$

where the positive constants c_k are chosen so that the integrals of both sides of (14) match. When k is large we see that c_k approaches 1. Moreover, we can normalize the solution ψ_k so that

$$\sup_M(\psi_k-\varphi)=\sup_M(\varphi-\psi_k).$$

Using (13) together with Kołodziej's stability result [2003] we obtain

$$\lim_{k\to\infty}\|\psi_k-\varphi\|_{L^\infty}=0. \tag{15}$$

Using Proposition 2 we can solve the equation

$$\frac{\partial\varphi_k}{\partial t}=\log\frac{(\omega+\sqrt{-1}\partial\overline{\partial}\varphi_k)^n}{\omega^n}+F(\varphi_k,z)-\log c_k, \tag{16}$$

with initial condition $\varphi_k|_{t=0}=\psi_k$ for a short time $t\in[0,T]$ independent of k, since by (13), (14) and (15) we have uniform bounds on the initial data $\sup|\psi_k|$ and $\sup|\dot{\varphi}_k(0)|$. As in [Song and Tian 2009] we have:

Lemma 6. *The sequence φ_k is a Cauchy sequence in $C^0([0,T]\times M)$, ie.*

$$\lim_{j,k\to\infty}\|\varphi_j-\varphi_k\|_{L^\infty([0,T]\times M)}=0.$$

Proof. Fix j,k and let $\mu=\varphi_j-\varphi_k$. Then

$$\frac{\partial\mu}{\partial t}=\log\frac{(\omega+\sqrt{-1}\partial\overline{\partial}\varphi_k+\sqrt{-1}\partial\overline{\partial}\mu)^n}{(\omega+\sqrt{-1}\partial\overline{\partial}\varphi_k)^n}+F(\varphi_j,z)-F(\varphi_k,z)+\log\frac{c_k}{c_j},$$

and $\mu|_{t=0}=\psi_j-\psi_k$. At any time given time t, the maximum of μ is achieved at some point $z\in M$, and at z we have

$$\frac{d\mu_{\max}}{dt}\leqslant F(\varphi_j(t,z),z)-F(\varphi_k(t,z),z)+\log\frac{c_k}{c_j}\leqslant\kappa|\mu(z)|+\log\frac{c_k}{c_j},$$

where κ is independent of j,k. Here and henceforth the derivative is interpreted as the limsup of the forward difference quotients at the points where it does not exist [Hamilton 1986, Lemma 3.5]. Similarly, at the point z' where the minimum of μ is achieved, we have

$$\frac{d\mu_{\min}}{dt}\geqslant-\kappa|\mu(z')|+\log\frac{c_k}{c_j}.$$

Putting these together we see that

$$\frac{d|\mu|_{\max}}{dt}\leqslant\kappa|\mu|_{\max}+\left|\log\frac{c_k}{c_j}\right|.$$

It follows that

$$\sup_{[0,T]\times M}|\varphi_j-\varphi_k|\leqslant e^{\kappa T}\left(\|\psi_j-\psi_k\|_{L^\infty(M)}+\frac{1}{\kappa}\left|\log\frac{c_k}{c_j}\right|\right)-\frac{1}{\kappa}\left|\log\frac{c_k}{c_j}\right|.$$

Now (15) and the fact that c_k converges to 1 imply the result. $\square$

Using this lemma we can define

$$\Phi=\lim_{j\to\infty}\varphi_j,$$

which is in $C^0([0,T]\times M)$. Moreover from Proposition 2 for any $\varepsilon>0$ we have uniform bounds on all derivatives of the φ_j for $t\in[\varepsilon,T]$, so in fact for all k we have

$$\lim_{j\to\infty}\|\Phi-\varphi_j\|_{C^k(M\times[\varepsilon,T])}=0.$$

From (6) we get

$$\sup_M|\dot{\varphi}_k(t)|<C\sup_M|\dot{\varphi}_k(0)|$$

for $t\in[0,T)$, but from (16) we have

$$\dot{\varphi}_k(0)=\log\frac{(\omega+\sqrt{-1}\partial\overline{\partial}\psi_k)^n}{\omega^n}+F(\psi_k,z)-\log c_k=F(\psi_k,z)-F(\varphi_k,z)-\log c_k,$$

which converges to zero when k goes to infinity. It follows that for any $t>0$ we have

$$\dot{\Phi}(t)=\lim_{j\to\infty}\dot{\varphi}_j(t)=0.$$

Hence Φ is constant on $(0,T]$, but since it is continuous on $[0,T]$ it follows that $\Phi(t)=\Phi(0)$ for all $t\leqslant T$. But $\Phi(0)$ is our solution φ of (12), whereas $\Phi(t)$ is smooth for $t>0$. Hence φ is smooth.

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TRAVELING WAVES FOR THE CUBIC SZEGŐ EQUATION ON THE REAL LINE

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We consider the cubic Szegő equation $i\partial tu = \Pi(|u|^2u)$ in the Hardy space $L^2_+(\mathbb{R})$ on the upper half-plane, where Π is the Szegő projector. It was first introduced by Gérard and Grellier as a toy model for totally nondispersive evolution equations. We show that the only traveling waves are of the form $C/(x-p)$, where $p \in \mathbb{C}$ with $\operatorname{Im} p < 0$. Moreover, they are shown to be orbitally stable, in contrast to the situation on the unit disk where some traveling waves were shown to be unstable.

1. Introduction

One of the most important properties in the study of nonlinear Schrödinger equations (NLS) is *dispersion*. It is often exhibited in the form of the Strichartz estimates of the corresponding linear flow. In case of the cubic NLS,

$$i\partial_t u + \Delta u = |u|^2 u, \quad (t,x) \in \mathbb{R} \times M, \tag{1-1}$$

Burq, Gérard, and Tzvetkov [Burq et al. 2005] observed that the dispersive properties are strongly influenced by the geometry of the underlying manifold M. Taking this idea further, Gérard and Grellier [2010b] remarked a lack of dispersion when M is a sub-Riemannian manifold (for example, the Heisenberg group). In this situation, many of the classical arguments used in the study of NLS no longer hold. As a consequence, even the problem of global well-posedness of (1-1) on a sub-Riemannian manifold still remains open.

Gérard and Grellier [2010a; 2010b] introduced a model of a nondispersive Hamiltonian equation called *the cubic Szegő equation.* (See (1-2) below.) The study of this equation is the first step toward understanding existence and other properties of smooth solutions of NLS in the absence of dispersion. Remarkably, the Szegő equation turned out to be completely integrable in the following sense. It possesses a Lax pair structure and an infinite sequence of conservation laws. Moreover, the dynamics can be approximated by a sequence of finite-dimensional completely integrable Hamiltonian systems. To illustrate the degeneracy of this completely integrable structure, several instability phenomena were established in [Gérard and Grellier 2010a].

Gérard and Grellier studied the Szegő equation on the circle $\mathbb{S}^1$. More precisely, solutions were considered to belong at all time to the Hardy space $L^2_+(\mathbb{S}^1)$ on the unit disk $\mathbb{D} = \{|z| < 1\}$. This is the space of L^2-functions on $\mathbb{S}^1$ with $\hat{f}(k) = 0$ for all $k < 0$. These functions can be extended as

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holomorphic functions on the unit disk. Several properties of the Hardy space on the unit disk naturally transfer to the Hardy space $L^2_+(\mathbb{R})$ on the upper half-plane $\mathbb{C}_+ = \{z; \operatorname{Im} z > 0\}$, defined by

$$L^2_+(\mathbb{R}) = \left\{ f \text{ holomorphic on } \mathbb{C}_+; \|g\|_{L^2_+(\mathbb{R})} := \sup_{y>0} \left(\int_{\mathbb{R}} |g(x+iy)|^2 \, dx \right)^{1/2} < \infty \right\}.$$

In view of the Paley–Wiener theorem, we identify this space of holomorphic functions on $\mathbb{C}_+$ with the space of its boundary values:

$$L^2_+(\mathbb{R}) = \{ f \in L^2(\mathbb{R}); \operatorname{supp} \hat{f} \subset [0, \infty) \}.$$

The transfer from $L^2_+(\mathbb{S}^1)$ to $L^2_+(\mathbb{R})$ is made by the usual conformal transformation

$$\omega : \mathbb{D} \to \mathbb{C}_+, \quad \omega(z) = i \frac{1+z}{1-z}.$$

However, the image of a solution of the Szegő equation on $\mathbb{S}^1$ under the conformal transformation is no longer a solution of the Szegő equation on $\mathbb{R}$. Therefore, we study the Szegő equation on $\mathbb{R}$ directly.

Endowing $L^2(\mathbb{R})$ with the usual scalar product $(u, v) = \int_{\mathbb{R}} u\bar{v}$, we define the Szegő projector $\Pi : L^2(\mathbb{R}) \to L^2_+(\mathbb{R})$ to be the projector onto the nonnegative frequencies:

$$\Pi(f)(x) = \frac{1}{2\pi} \int_0^\infty e^{ix\xi} \hat{f}(\xi) \, d\xi.$$

For $u \in L^2_+(\mathbb{R})$, we consider *the Szegő equation on the real line*:

$$i\partial_t u = \Pi(|u|^2 u), \quad x \in \mathbb{R}. \tag{1-2}$$

This is a Hamiltonian evolution associated to the Hamiltonian

$$E(u) = \int_{\mathbb{R}} |u|^4 \, dx$$

defined on $L^4_+(\mathbb{R})$. From this structure, we obtain the formal conservation law

$$E(u(t)) = E(u(0)).$$

The invariance under translations and under modulations provides two more conservation laws,

$$Q(u(t)) = Q(u(0)) \quad \text{and} \quad M(u(t)) = M(u(0)),$$

where

$$Q(u) = \int_{\mathbb{R}} |u|^2 \, dx \quad \text{and} \quad M(u) = \int_{\mathbb{R}} \bar{u} Du \, dx, \ \text{ with } D = -i\partial_x.$$

Now, we define the Sobolev spaces $H^s_+(\mathbb{R})$ for $s \geq 0$:

$$H^s_+(\mathbb{R}) = \left\{ h \in L^2_+(\mathbb{R}); \|h\|_{H^s_+} := \left(\frac{1}{2\pi} \int_0^\infty (1+|\xi|^2)^s |\hat{h}(\xi)|^2 \, d\xi \right)^{1/2} < \infty \right\}.$$

Similarly, we define the homogeneous Sobolev norm for $h \in \dot{H}^s_+$ by

$$\|h\|_{\dot{H}^s_+} := \left(\frac{1}{2\pi}\int_0^\infty |\xi|^{2s}|\hat{h}(\xi)|^2\right)^{1/2} < \infty.$$

Slight modifications of the proof of the corresponding result in [Gérard and Grellier 2010a] lead to this well-posedness result:

Theorem 1.1. *The cubic Szegő equation* (1-2) *is globally well-posed in $H^s_+(\mathbb{R})$ for $s \geq \frac{1}{2}$. That is, given $u_0 \in H^{1/2}_+$, there exists a unique global-in-time solution $u \in C(\mathbb{R}; H^{1/2}_+)$ of* (1-2) *with initial condition u_0. Moreover, if $u_0 \in H^s_+$ for some $s > \frac{1}{2}$, then $u \in C(\mathbb{R}; H^s_+)$.*

In this paper, we concentrate on the study of traveling waves. The two main goals are the classification of traveling waves and their stability. As a result, we show that the situation on the real line is essentially different from that on the circle.

A solution for the cubic Szegő equation on the real line (1-2) is called a *traveling wave* if there exist $c, \omega \in \mathbb{R}$ such that

$$u(t,z) = e^{-i\omega t}u_0(z-ct), \quad z \in \mathbb{C}_+ \cup \mathbb{R},\ t \in \mathbb{R} \tag{1-3}$$

for some $u_0 \in H^{1/2}_+(\mathbb{R})$. Note that a solution to (1-2) in $H^{1/2}_+(\mathbb{R})$ has a natural extension onto $\mathbb{C}_+$, and we have used this viewpoint in (1-3). Substituting (1-3) into (1-2), we see that u_0 satisfies on $\mathbb{R}$ the equation

$$cDu_0 + \omega u_0 = \Pi(|u_0|^2 u_0). \tag{1-4}$$

In the following, we use the simpler notation u instead of u_0 when we study time-independent problems. From (1-4), we see that traveling waves with nonzero velocity, $c \neq 0$, have good regularity. Indeed, we prove that $u \in H^s_+(\mathbb{R})$ for all $s \geq 0$ in Lemma 3.1. In particular, by Sobolev embedding theorem, we have $u \in L^p_+(\mathbb{R})$ for $2 \leq p \leq \infty$. On the other hand, (1-4) yields in Lemma 4.1 that there exist no nontrivial stationary waves, i.e. traveling waves of velocity $c = 0$, in L^2_+.

Now, we present our main results:

Theorem 1.2. *A function $u \in C(\mathbb{R}, H^{1/2}_+(\mathbb{R}))$ is a traveling wave if and only if there exist $C, p \in \mathbb{C}$ with* $\operatorname{Im}\ p < 0$ *such that*

$$u(0,z) = \frac{C}{z-p}. \tag{1-5}$$

Theorem 1.3. *Let $a > 0$, $r > 0$, and consider the cylinder*

$$C(a,r) = \left\{\frac{\alpha}{z-p};\, |\alpha| = a,\ \operatorname{Im} p = -r\right\}.$$

Let $\{u_0^n\} \subset H^{1/2}_+$ with

$$\inf_{\phi \in C(a,r)} \|u_0^n - \phi\|_{H^{1/2}_+} \to 0 \text{ as } n \to +\infty,$$

and let u^n denote the solution to (1-2) *with initial data u_0^n. Then*

$$\sup_{t\in\mathbb{R}} \inf_{\phi \in C(a,r)} \|u^n(t,x) - \phi(x)\|_{H^{1/2}_+} \to 0.$$

Let us compare our results to those in [Gérard and Grellier 2010a]. In the case of the Szegő equation on $\mathbb{S}^1$, the nontrivial stationary waves ($c = 0$) are finite Blaschke products of the form

$$\alpha \prod_{j=1}^{N} \frac{z - p_j}{1 - \bar{p}_j z},$$

where $|\alpha|^2 = \omega$, $N \in \mathbb{N}$, and $p_1, p_2, \dots, p_N \in \mathbb{D}$, and the traveling waves with nonzero velocity are rational functions of the form

$$\frac{C z^l}{z^N - p}, \tag{1-6}$$

where $N \in \mathbb{N}$, $l \in \{0, 1, \dots, N-1\}$, $C, p \in \mathbb{C}$, and $|p| > 1$. Moreover, instability phenomena were displayed for some of the above traveling waves. For the cubic Szegő equation on $\mathbb{R}$, Theorems 1.2 and 1.3 state that there exist fewer traveling waves — corresponding to $N = 1$ and $l = 0$ in (1-6) — and that there is no instability phenomenon.

The proof of Theorem 1.2 involves arguments from several areas of analysis: a Kronecker-type theorem, scattering theory, existence of a Lax pair structure, a theorem by Lax on invariant subspaces of the Hardy space, and canonical factorization of Beurling–Lax inner functions. We now introduce the main notions and known results, and briefly describe the strategy of the proof.

As in [Gérard and Grellier 2010a], an important property of the Szegő equation on $\mathbb{R}$ is the existence of a Lax pair structure. Using the Szegő projector, we first define two important classes of operators on L^2_+: *the Hankel and Toeplitz operators*. We use these operators to find a Lax pair. See Proposition 1.4.

A Hankel operator $H_u : L^2_+ \to L^2_+$ of symbol $u \in H^{1/2}_+$ is defined by

$$H_u(h) = \Pi(u\bar{h}).$$

H_u is $\mathbb{C}$-antilinear and satisfies

$$(H_u(h_1), h_2) = (H_u(h_2), h_1). \tag{1-7}$$

In Lemma 3.5 below we prove that H_u is a Hilbert–Schmidt operator of Hilbert–Schmidt norm

$$\frac{1}{\sqrt{2\pi}} \|u\|_{\dot{H}^{1/2}}.$$

A Toeplitz operator $T_b : L^2_+ \to L^2_+$ of symbol $b \in L^\infty(\mathbb{R})$ is defined by

$$T_b(h) = \Pi(bh).$$

T_b is $\mathbb{C}$-linear. Moreover, T_b is self-adjoint if and only if b is real-valued.

Proposition 1.4. *Let $u \in C(\mathbb{R}; H^s_+)$ for some $s > \frac{1}{2}$. The cubic Szegő equation* (1-2) *is equivalent to the evolution equation*

$$\frac{d}{dt} H_u = [B_u, H_u], \tag{1-8}$$

where $B_u = \frac{i}{2} H_u^2 - i T_{|u|^2}$. In other words, the pair (H_u, B_u) is a Lax pair for the cubic Szegő equation on the real line.

The proof of Proposition 1.4 follows the same lines as that of the corresponding result on $\mathbb{S}^1$ in [Gérard and Grellier 2010a], and is based on the identity

$$H_{\Pi(|u|^2u)} = T_{|u|^2} H_u + H_u T_{|u|^2} - H_u^3. \tag{1-9}$$

Combining (1-4) and (1-9), we deduce that if u is a traveling wave with $c \neq 0$, then the identity

$$A_u H_u + H_u A_u + \frac{\omega}{c} H_u + \frac{1}{c} H_u^3 = 0, \tag{1-10}$$

holds, where

$$A_u = D - \frac{1}{c} T_{|u|^2}. \tag{1-11}$$

In Section 2, we prove a Kronecker-type theorem for the Hardy space $L^2_+(\mathbb{R})$, where we classify all the symbols u such that the operator H_u has finite rank. The classical theorem for $L^2_+(\mathbb{S}^1)$ is due to Kronecker. For a proof, see [Gérard and Grellier 2010a].

We prove Theorem 1.2 in Section 4. We first prove that all traveling waves are rational functions. On $\mathbb{S}^1$, this follows easily from the Kronecker theorem and the fact that the operator A_u has discrete spectrum. On $\mathbb{R}$, however, it turns out that A_u has continuous spectrum. Therefore, we use scattering theory to study the spectral properties of A_u in detail in Section 3. More precisely, we show that the generalized wave operators $\Omega^{\pm}(D, A_u)$, rigorously defined by (3-1) below, exist and are complete. As a result, we obtain that

$$\mathcal{H}_{\mathrm{ac}}(A_u) \subset \operatorname{Ker} H_u,$$

where $\mathcal{H}_{\mathrm{ac}}(A_u)$ is the absolutely continuous subspace of A_u. The subspace $\operatorname{Ker} H_u$ plays an important role in our analysis. More precisely, it turns out to be invariant under multiplication by $e^{i\alpha x}$, for all $\alpha \geq 0$. Therefore, applying a theorem by Lax (Proposition 4.4) on invariant subspaces, it results that

$$\operatorname{Ker} H_u = \phi L^2_+,$$

where ϕ is an inner function in the sense of Beurling and Lax, i.e., a bounded holomorphic function on $\mathbb{C}_+$ such that $|\phi(x)| = 1$ for all $x \in \mathbb{R}$. Using the Lax pair structure and the identity (1-10), we show that ϕ satisfies the simple equation

$$cD\phi = |u|^2\phi.$$

However, as an inner function, ϕ satisfies a canonical factorization (4-3). From this, it follows that ϕ belongs to a special class of inner functions, the finite Blaschke products, i.e.,

$$\phi(z) = \prod_{j=1}^{N} \frac{z - \lambda_j}{z - \bar{\lambda}_j},$$

where $N \in \mathbb{N}$ and $\operatorname{Im} \lambda_j > 0$ for all $j = 1, 2, \ldots, N$. The Kronecker-type theorem then yields that the traveling wave u is a rational function. In the case of $\mathbb{S}^1$, the natural shift, multiplication by e^{ix}, was used in concluding traveling waves are of the form (1-6). In our case, we use the "infinitesimal" shift, multiplication by x, to show that traveling waves are of the form (1-5).

Finally, we prove Theorem 1.3 in Section 5. The orbital stability of traveling waves is a consequence of the fact that traveling waves are ground states for the following inequality, an analogue of the sharp Gagliardo–Nirenberg inequality given in [Weinstein 1982].

Proposition 1.5. *For all* $u \in H^{1/2}_+(\mathbb{R})$, *the following Gagliardo–Nirenberg inequality holds*:

$$\|u\|_{L^4} \le \frac{1}{\sqrt[4]{\pi}} \|u\|^{1/2}_{L^2} \|u\|^{1/2}_{\dot{H}^{1/2}_+}, \tag{1-12}$$

or, *equivalently*,

$$E \le \frac{1}{\pi} M Q.$$

Equality holds if and only if $u = \dfrac{C}{x-p}$, *where* $C, p \in \mathbb{C}$ *with* $\operatorname{Im} p < 0$.

Remark 1.6. Using Proposition 1.5, one can verify that the functions $u = C/(x-p)$, with $\operatorname{Im} p < 0$, are indeed initial data for traveling waves. More precisely, since they are minimizers of the functional

$$v \in H^{1/2}_+ \mapsto M(v)Q(v) - \pi E(v),$$

the differential of this functional at u is zero. Thus,

$$\tfrac{1}{2} Q(u) Du + \tfrac{1}{2} M(u) u - \pi \Pi(|u|^2 u) = 0.$$

Consequently, u is a solution of (1-4) with

$$c = \frac{Q(u)}{2\pi} = \frac{|C|^2}{-2 \operatorname{Im} p}, \quad \omega = \frac{M(u)}{2\pi} = \frac{|C|^2}{4(\operatorname{Im} p)^2},$$

and hence it is an initial datum for a traveling wave.

In the case of $\mathbb{S}^1$, the Gagliardo–Nirenberg inequality suffices to conclude the stability of the traveling waves with $N = 1$. However, in the case of $\mathbb{R}$, we need to use in addition a concentration-compactness argument. This concentration-compactness argument, which first appeared in [Cazenave and Lions 1982], was refined and turned into profile decomposition theorems by Gérard [1998] and later by Hmidi and Keraani [2006]. We use it in the form of Proposition 5.1, a profile decomposition theorem for bounded sequences in $H^{1/2}_+$.

We conclude this introduction by presenting two open problems. Here, we use the term soliton instead of traveling wave, so that we put into light several connections with existing works. The first problem is the soliton resolution, which consists in writing any solution as a superposition of solitons and radiation. For the KdV equation, this property was rigorously stated in [Eckhaus and Schuur 1983] for initial data to which the Inverse Scattering Transform applies. Therefore, for the Szegő equation, one needs to solve inverse spectral problems for the Hankel operators and also find explicit action angle coordinates.

The second open problem is the interaction of solitons with external potentials. Consider the Szegő equation with a linear potential, where initial data are taken to be of the form (1-5). As in [Holmer and Zworski 2008] and [Perelman 2009], it would be interesting to investigate if solutions of the perturbed Szegő equation can be approximated by traveling wave solutions to the original Szegő equation (1-2).

2. A Kronecker-type theorem

A theorem by Kronecker asserts in the setting of $\mathbb{S}^1$ that the set of symbols u such that H_u is of rank N is precisely a $2N$-dimensional complex submanifold of $L^2_+(\mathbb{S}^1)$ containing only rational functions. In this section, we prove the analogue of this. For a different proof of a similar result on some Hankel operators on $L^2_+(\mathbb{R})$ defined in a slightly different way, see [Peller 2003, Lemma 8.12, p. 54].

Definition. Let $N \in \mathbb{N}^*$. We denote by $\mathcal{M}(N)$ the set of rational functions of the form

$$\frac{A(z)}{B(z)},$$

where $A \in \mathbb{C}_{N-1}[z]$, $B \in \mathbb{C}_N[z]$, $0 \leq \deg(A) \leq N-1$, $\deg(B) = N$, $B(0) = 1$, $B(z) \neq 0$, for all $z \in \mathbb{C}_+ \cup \mathbb{R}$, and A and B have no common factors.

Theorem 2.1. *A function u belongs to $\mathcal{M}(N)$ if and only if the Hankel operator H_u has complex rank N.*

Moreover, if $u \in \mathcal{M}(N)$ is of the form $u(z) = A(z)/B(z)$, where $B(z) = \prod_{j=1}^{J}(z-p_j)^{m_j}$ with $\sum_{j=1}^{J} m_j = N$ and $\operatorname{Im} p_j < 0$ *for all $j = 1, 2, \ldots, J$, then the range of H_u is given by*

$$\operatorname{Ran} H_u = \operatorname{span}_{\mathbb{C}}\left\{\frac{1}{(z-p_j)^m}; 1 \leq m \leq m_j\right\}_{j=1}^{J} \tag{2-1}$$

Proof. The theorem will follow from two implications:

(i) $u \in \mathcal{M}(N) \Longrightarrow \operatorname{rk}(H_u) \leq N$.

(ii) $\operatorname{rk}(H_u) = N \Longrightarrow u \in \mathcal{M}(N)$.

Let us first prove (i). Let $u \in \mathcal{M}(N)$, i.e., u is a linear combination of terms $\dfrac{1}{(z-p)^m}$, where $\operatorname{Im} p < 0$, $1 \leq m \leq m_p$, and $\sum m_p = N$. Computing the integral

$$\int_{\mathbb{R}} \frac{e^{-ix\xi}}{(x-p)^m}\, dx,$$

using the residue theorem, we obtain that $\hat{u}(\xi) = 0$ for all $\xi \leq 0$ and $\hat{u}(\xi)$ is a linear combination of terms $\xi^{m-1} e^{-ip\xi}$, with $1 \leq m \leq m_p$, for $\xi > 0$.

Given $h \in L^2_+$, we have $\widehat{H_u(h)}(\xi) = 0$ for $\xi < 0$. For $\xi > 0$, we have

$$\begin{aligned}
\widehat{H_u(h)}(\xi) &= \frac{1}{2\pi}\int_{-\infty}^{0} \hat{u}(\xi-\eta)\hat{\bar{h}}(\eta)\, d\eta = \frac{1}{2\pi}\int_{0}^{\infty} \hat{u}(\xi+\eta)\overline{\hat{h}}(\eta)\, d\eta \\
&= \sum_{\substack{1 \leq m \leq m_p \\ \sum m_p = N}} c_{m,p}\left(\sum_{k=0}^{m-1} C_{m-1}^{k} \xi^{m-1-k}\int_0^\infty \eta^k \overline{\hat{h}}(\eta) e^{-ip\eta}\, d\eta\right) e^{-ip\xi} \\
&= \sum_{\substack{1 \leq m \leq m_p \\ \sum m_p = N}} \tilde{d}_{m,p}(u,h)\xi^{m-1}e^{-ip\xi} = \sum_{\substack{1 \leq m \leq m_p \\ \sum m_p = N}} d_{m,p}(u,h)\left(\frac{1}{(x-p)^m}\right)^{\wedge}(\xi),
\end{aligned}$$

where $c_{m,p}$, $\tilde{d}_{m,p}$, $d_{m,p}$ are constants depending on p and m. Hence,

$$H_u(h)(x) = \sum_{\substack{1\le m\le m_p \\ \sum m_p = N}} \frac{d_{m,p}(u,h)}{(x-p)^m} \tag{2-2}$$

and $\mathrm{rk}(H_u) \le N$.

Let us now prove (ii). Assume that $\mathrm{rank}(H_u) = N$, so the range of H_u, Ran H_u, is a $2N$-dimensional real vector space. As H_u is $\mathbb{C}$-antilinear, one can choose a basis of Ran H_u of eigenvectors of H_u in the following way:

$$\{v_1, iv_1, \dots, v_N, iv_N\,;\ H_u(v_j) = \lambda_j v_j, \lambda_j > 0,\ j = 1, 2, \dots, N\}$$

Let $w_j = \sqrt{\lambda_j}\, v_j$. If $h \in L^2_+$, then by Parseval's identity we have

$$\begin{aligned} H_u(h) &= \sum_{j=1}^N (H_u(h), v_j) v_j + \sum_{j=1}^N (H_u(h), iv_j) iv_j = 2\sum_{j=1}^N (H_u(h), v_j) v_j = 2\sum_{j=1}^N (H_u(v_j), h) v_j \\ &= 2\sum_{j=1}^N (\lambda_j v_j, h) v_j = 2\sum_{j=1}^N (w_j, h) w_j = \frac{1}{\pi}\sum_{j=1}^N \Big(\int_0^\infty \hat{w}_j(\eta)\bar{\hat{h}}(\eta)\, d\eta\Big) w_j. \end{aligned}$$

Consequently,

$$\widehat{H_u(h)}(\xi) = \frac{1}{2\pi}\mathbf{1}_{\xi\ge 0}\int_0^\infty \hat{u}(\xi+\eta)\bar{\hat{h}}(\eta)\, d\eta = \frac{1}{\pi}\mathbf{1}_{\xi\ge 0}\sum_{j=1}^N \int_0^\infty \hat{w}_j(\eta)\hat{w}_j(\xi)\bar{\hat{h}}(\eta)\, d\eta,$$

and hence,

$$\mathbf{1}_{\xi\ge 0}\int_0^\infty \Big(\hat{u}(\xi+\eta) - 2\sum_{j=1}^N \hat{w}_j(\eta)\hat{w}_j(\xi)\Big)\bar{\hat{h}}(\eta)\, d\eta = 0,$$

for all $h \in L^2_+$. Therefore, for all $\xi, \eta \ge 0$, we have

$$\hat{u}(\xi+\eta) = 2\sum_{j=1}^N \hat{w}_j(\eta)\hat{w}_j(\xi). \tag{2-3}$$

Let $L > 2N+1$ be an even integer and let ϕ be the probability density function of the chi-square distribution defined by

$$\phi(\xi) = \begin{cases} 2^{-L/2}\Gamma\Big(\dfrac{L}{2}\Big)^{-1}\xi^{(L/2)-1}e^{-\xi/2} & \text{if } \xi \ge 0, \\ 0 & \text{if } \xi < 0, \end{cases}$$

where Γ is the gamma function. Then, its Fourier transform is

$$\widehat{\phi}(x) = (1+2ix)^{-L/2}.$$

Notice that $\phi \in H^N(\mathbb{R})$ since

$$\|\phi\|_{H^N}^2 = \int_{\mathbb{R}} \frac{\langle x\rangle^{2N}}{|1+2ix|^L}\,dx,$$

which is convergent if and only if $2N - L < -1$.

Let $\langle \theta, \psi\rangle = \int_{\mathbb{R}} \theta(x)\psi(x)$ for all $\theta \in H^{-N}(\mathbb{R})$ and $\psi \in H^N(\mathbb{R})$. Consider the matrix A_ϕ defined by

$$\begin{pmatrix} \langle \hat{w}_1, \phi\rangle & \langle \hat{w}_1', \phi\rangle & \cdots & \langle \hat{w}_1^{(N)}, \phi\rangle \\ \langle \hat{w}_2, \phi\rangle & \langle \hat{w}_2', \phi\rangle & \cdots & \langle \hat{w}_2^{(N)}, \phi\rangle \\ \vdots & \vdots & \ddots & \vdots \\ \langle \hat{w}_N, \phi\rangle & \langle \hat{w}_N', \phi\rangle & \cdots & \langle \hat{w}_N^{(N)}, \phi\rangle \end{pmatrix}.$$

Since $\mathrm{rk}(A_\phi) \le N$, it results that there exists $(c_0, c_1, \dots, c_N) \ne 0$ such that

$$\Big\langle \sum_{k=0}^N c_k \hat{w}_j^{(k)}, \phi \Big\rangle = 0,$$

for all $j = 1, 2, \dots, N$. Then, since $\operatorname{supp}\phi \subset [0,\infty)$ and by (2-3), we have for all $\eta \ge 0$ that

$$\begin{aligned} \sum_{k=0}^N \Big\langle c_k \hat{u}^{(k)}(\xi), \phi(\xi-\eta)\Big\rangle_\xi &= \sum_{k=0}^N \Big\langle c_k \hat{u}^{(k)}(\xi+\eta), \phi(\xi)\Big\rangle_\xi = \sum_{k=0}^N (-1)^k c_k \int_0^\infty \hat{u}(\xi+\eta)\phi^{(k)}(\xi)d\xi \\ &= 2\sum_{k=0}^N (-1)^k c_k \int_0^\infty \Big(\sum_{j=1}^N \hat{w}_j(\eta)\hat{w}_j(\xi)\Big)\phi^{(k)}(\xi)d\xi \\ &= 2\sum_{j=1}^N \hat{w}_j(\eta) \sum_{k=0}^N c_k \Big\langle \hat{w}_j^{(k)}(\xi), \phi(\xi)\Big\rangle = 0. \end{aligned}$$

Set $T = \sum_{k=0}^N c_k \hat{u}^{(k)}$. Then $T \in H^{-N}$ and $\operatorname{supp} T \in [0,\infty)$. We have just proved that for all $\eta \ge 0$

$$\begin{aligned} 0 = \langle T, \phi(\cdot-\eta)\rangle &= \int_{\mathbb{R}} T(\xi)\phi(\xi-\eta)d\xi = \int_{\mathbb{R}} T(\xi)\Big(\int_{\mathbb{R}} \frac{e^{ix(\xi-\eta)}}{(1+2ix)^{L/2}}dx\Big)d\xi \\ &= \int_{\mathbb{R}} \Big(\int_{\mathbb{R}} T(\xi)e^{ix\xi}d\xi\Big)\frac{e^{-ix\eta}}{(1+2ix)^{L/2}}dx = \int_{\mathbb{R}} \mathscr{F}^{-1}T(x)\frac{e^{-ix\eta}}{(1+2ix)^{L/2}}dx. \end{aligned}$$

Seting $R(x) := \frac{1}{(1+2ix)^{L/2}}\mathscr{F}^{-1}T(x)$, we have $\hat{R} \in H^{L/2-N}(\mathbb{R}) \subset H^{1/2}(\mathbb{R})$ and

$$0 = \int_{\mathbb{R}} R(x)e^{-ix\eta}dx = \hat{R}(\eta) \quad \text{for all } \eta \ge 0.$$

Thus $\operatorname{supp}\hat{R} \subset (-\infty, 0]$. By the definition of R, $(1-2D_\xi)^{L/2}\hat{R}(\xi) = T(\xi)$. Since the left hand-side is supported on $(-\infty,0]$ and the right hand-side is supported on $[0,\infty)$, we deduce that $\operatorname{supp} T \subset 0$. In particular, $T_{|\xi>0} = 0$. This yields that $\hat{u}_{|\xi>0}$ is a weak solution on $(0,\infty)$ of the linear ordinary differential equation

$$\sum_{k=0}^{N} c_k v^{(k)}(\xi) = 0.$$

Then, by [Hörmander 1990, Theorem 4.4.8, p. 115], we have $\hat{u}_{|\xi>0} \in C^N((0,\infty))$; further, $\hat{u}_{|\xi>0}$ is a classical solution of this equation, and therefore it is a linear combination of terms

$$\xi^{m-1} e^{q\xi},$$

where $q \in \mathbb{C}$ is a root of the polynomial $P(X) = \sum_{k=0}^{N} c_k X^k$ with multiplicity m_q, $1 \le m \le m_q$, and $\sum_q m_q = N$. Note that we must have $\operatorname{Re} q < 0$, because $u \in L^2_+(\mathbb{R})$. Therefore we will set $q = -ip$, with $\operatorname{Im} p < 0$, and obtain that $\hat{u}(\xi)$ is a linear combination of terms $\xi^{m-1} e^{-ip\xi}$ for $\xi > 0$. By the hypothesis $u \in L^2_+(\mathbb{R})$, we obtain $\hat{u}(\xi) = 0$ for $\xi \le 0$. Hence, for all $\xi \in \mathbb{R}$, $\hat{u}(\xi)$ is a linear combination of $((x-p)^{-m})^\wedge(\xi)$, with $1 \le q \le m_q$ and $\sum m_q = N$. Thus $u \in \mathcal{M}(N')$ for some $N' \le N$. If $N' < N$, implication (i) above yields $\operatorname{rk}(H_u) \le N'$, contradicting our assumption. In conclusion, $u \in \mathcal{M}(N)$.

Finally, when $u \in \mathcal{M}(N)$ we have $\operatorname{rk}(H_u) = N$ and (2-2), and thus (2-1) follows. □

As a consequence of (2-1) we make the following remark.

Remark 2.2. If $u \in \mathcal{M}(N)$, then $u \in \operatorname{Ran} H_u$.

3. Spectral properties of the operator A_u for a traveling wave u

Let us first recall the definition and the basic properties of the generalized wave operators, which are the main objects in scattering theory. We refer to [Reed and Simon 1979, Chapter XI] for more details.

Let A and B be two self-adjoint operators on a Hilbert space $\mathcal{H}$. The basic principle of scattering theory is to compare the free dynamics corresponding to e^{-iAt} and e^{-iBt}. The fact that $e^{-iBt}\phi$ "looks asymptotically free" as $t \to -\infty$, with respect to A, means that there exists $\phi_+ \in \mathcal{H}$ such that

$$\lim_{t\to-\infty} \|e^{-iBt}\phi - e^{-itA}\phi_+\| = 0,$$

or, equivalently,

$$\lim_{t\to-\infty} \|e^{iAt}e^{-itB}\phi - \phi_+\| = 0.$$

Hence, we reduced ourselves to the problem of the existence of a strong limit. Let $\mathcal{H}_{\mathrm{ac}}(B)$ be the absolutely continuous subspace for B and let $P_{\mathrm{ac}}(B)$ be the orthogonal projection onto this subspace. In the definition of the generalized wave operators we have $\phi \in \mathcal{H}_{\mathrm{ac}}(B)$.

We say that the generalized wave operators exist if the following strong limits exist:

$$\Omega^{\pm}(A,B) = \lim_{t\to\mp\infty} e^{itA}e^{-itB}P_{\mathrm{ac}}(B). \tag{3-1}$$

The wave operators $\Omega^{\pm}(A,B)$ are partial isometries with initial subspace $\mathcal{H}_{\mathrm{ac}}(B)$ and with values in $\operatorname{Ran}\Omega^{\pm}(A,B)$. Moreover, $\operatorname{Ran}\Omega^{\pm}(A,B) \subset \mathcal{H}_{\mathrm{ac}}(A)$. If $\operatorname{Ran}\Omega^{\pm}(A,B) = \mathcal{H}_{\mathrm{ac}}(A)$, we say that the generalized wave operators are complete. Lastly, we note that

$$A\Omega^{\pm}(A,B) = \Omega^{\pm}(A,B)B. \tag{3-2}$$

Lemma 3.1. *If $u \in H^{1/2}_+$ is a traveling wave, then $u \in H^s_+(\mathbb{R})$ for all $s \geq 0$. In particular, by Sobolev embedding theorem, we have $u \in L^p(\mathbb{R})$ for $2 \leq p \leq \infty$.*

Proof. Because $u \in H^{1/2}(\mathbb{R})$, the Sobolev embedding theorem yields $u \in L^p(\mathbb{R})$, for all $2 \leq p < \infty$. Therefore $|u|^2 u \in L^2(\mathbb{R})$ and thus $\Pi(|u|^2 u) \in L^2_+$. Using equation (1-4), namely

$$cDu + \omega u = \Pi(|u|^2 u),$$

we deduce that $Du \in L^2_+$. Consequently, $u \in H^1_+$ and by Sobolev embedding theorem we have $u \in L^\infty(\mathbb{R})$. Then $u^2 D\bar{u}, |u|^2 Du \in L^2(\mathbb{R})$. Applying the operator D to both sides of (1-4), we obtain $D^2 u \in L^2(\mathbb{R})$ and hence $u \in H^2_+$. Iterating this argument infinitely many times, the conclusion follows. □

Proposition 3.2. *Let u be a traveling wave. Then, $(A_u + i)^{-1} - (D + i)^{-1}$ is a trace class operator.*

Proof. We prove first that for all $f \in L^2(\mathbb{R})$, the operator $(D + i)^{-1} f$, defined on $L^2(\mathbb{R})$ by

$$\big((D + i)^{-1} f\big)h(x) = (D + i)^{-1}(fh)(x)$$

is Hilbert–Schmidt. Denote by $\mathcal{F}$ the Fourier transform. In view of the isomorphism of $L^2(\mathbb{R})$ induced by the Fourier transform, $(D + i)^{-1} f$ is a Hilbert–Schmidt operator if and only if $\mathcal{F}(D + i)^{-1} f$ is one. The latter is an integral operator of kernel

$$K(\xi, \eta) = \frac{1}{2\pi} \cdot \frac{1}{\xi + i} \hat{f}(\xi - \eta).$$

Indeed,

$$\mathcal{F}\big((D + i)^{-1} fh\big)(\xi) = \frac{1}{2\pi} \cdot \frac{1}{\xi + i} \widehat{fh}(\xi) = \frac{1}{2\pi} \int_{\mathbb{R}} \frac{1}{\xi + i} \hat{f}(\xi - \eta)\hat{h}(\eta)\, d\eta = \int_{\mathbb{R}} K(\xi, \eta)\hat{h}(\eta)\, d\eta.$$

Therefore, it is Hilbert–Schmidt if and only if $K(\xi, \eta) \in L^2_{\xi,\eta}(\mathbb{R} \times \mathbb{R})$. By the change of variables $\eta \mapsto \zeta = \xi - \eta$ we have

$$\|K(\xi, \eta)\|^2_{L^2_{\xi,\eta}} = \frac{1}{4\pi^2} \int_{\mathbb{R}} \frac{d\xi}{\xi^2 + 1} \int_{\mathbb{R}} |\hat{f}(\zeta)|^2\, d\zeta = C\|f\|^2_{L^2} < \infty.$$

Hence $(D + i)^{-1} f$ is a Hilbert–Schmidt operator and so is $\bar{f}(D + i)^{-1}$, its adjoint. According to Lemma 3.1, $u \in L^\infty(\mathbb{R})$ and thus $|u|^2 \in L^2(\mathbb{R})$. Taking $f = |u|^2$ and $f = u$, we conclude that the operators $(D + i)^{-1}|u|^2$, $(D + i)^{-1}u$, and $\bar{u}(D + i)^{-1}$ are all Hilbert–Schmidt.

We write

$$\begin{aligned} (A_u + i)^{-1} - (D + i)^{-1} &= (D + i)^{-1}(D - A_u)(A_u + i)^{-1} \\ &= \frac{1}{c}(D + i)^{-1} T_{|u|^2}(A_u + i)^{-1} \\ &= \frac{1}{c}\Pi(D + i)^{-1}|u|^2(A_u + i)^{-1} = L(A_u + i)^{-1}, \end{aligned}$$

where $L = \frac{1}{c}\Pi(D + i)^{-1}|u|^2$. Note that L is a Hilbert–Schmidt operator since it is the composition of the bounded operator $\frac{1}{c}\Pi : L^2(\mathbb{R}) \to L^2_+$ with the Hilbert–Schmidt operator $(D + i)^{-1}|u|^2$. Finally, we write, using the latter formula twice

$$\begin{aligned}(A_u+i)^{-1}-(D+i)^{-1} &= L(L(A_u+i)^{-1}+(D+i)^{-1})\\ &= L\circ L\circ(A_u+i)^{-1}+\frac{1}{c}\Pi(D+i)^{-1}u\circ\bar{u}(D+i)^{-1}.\end{aligned}$$

We obtain that $(A_u+i)^{-1}-(D+i)^{-1}$ is a trace class operator since the composition of two Hilbert–Schmidt operators is a trace class operator. □

Corollary 3.3. *If u is a traveling wave, the wave operators $\Omega^{\pm}(D, A_u)$ exist and are complete.*

Proof. This easily follows from Kuroda–Birman theorem [Reed and Simon 1979, Theorem XI.9]: *Let A and B be two self-adjoint operators on a Hilbert space such that $(A+i)^{-1}-(B+i)^{-1}$ is a trace class operator. Then $\Omega^{\pm}(A, B)$ exist and are complete.* □

Corollary 3.4. *If u is a traveling wave, then $\sigma_{\mathrm{ac}}(A_u)=[0,+\infty)$.*

Proof. Since $\Omega^{\pm}(D, A_u)$ are complete, it results that they are isometries from $\mathscr{H}_{\mathrm{ac}}(A_u)$ onto $\mathscr{H}_{\mathrm{ac}}(D)=L^2_+$. By (3-2), we then have

$$A_{u|_{\mathscr{H}_{\mathrm{ac}}(A_u)}}=[\Omega^{\pm}(D,A_u)_{|_{\mathscr{H}_{\mathrm{ac}}(A_u)}}]^{-1}D\Omega^{\pm}(D,A_u)_{|_{\mathscr{H}_{\mathrm{ac}}(A_u)}}.$$

Consequently, $\sigma_{\mathrm{ac}}(A_u)=\sigma_{\mathrm{ac}}(D)=[0,+\infty)$. □

Our main goal in the following is to prove that $\mathscr{H}_{\mathrm{ac}}(A_u)\subset \operatorname{Ker} H_u$. As we will see below, it is enough to prove that $\left[\Omega^+(D,A_u)H_u^2\right](\mathscr{H}_{\mathrm{ac}}(A_u))=0$.

Lemma 3.5. *H_u is a Hilbert–Schmidt operator on $L^2_+(\mathbb{R})$ of Hilbert–Schmidt norm $\dfrac{1}{\sqrt{2\pi}}\|u\|_{\dot{H}^{1/2}_+}$.*

Proof. Denote by $\|T\|_{HS}$ the Hilbert–Schmidt norm of a Hilbert–Schmidt operator T. By (2-2), we have

$$\widehat{H_u(h)}(\xi)=\frac{1}{2\pi}\mathbf{1}_{\xi\geq 0}\int_0^\infty \hat{u}(\xi+\eta)\bar{\hat{h}}(\eta)\,d\eta.$$

Then, we obtain

$$\begin{aligned}H_u(h)(x)&=\frac{1}{4\pi^2}\int_0^\infty\!\!\int_0^\infty e^{ix\xi}\hat{u}(\xi+\eta)\bar{\hat{h}}(\eta)\,d\eta d\xi\\ &=\frac{1}{4\pi^2}\int_{\mathbb{R}}\left(\int_0^\infty\!\!\int_0^\infty e^{ix\xi}e^{iy\eta}\hat{u}(\xi+\eta)\,d\eta\,d\xi\right)\bar{h}(y)\,dy.\end{aligned}$$

Using the fact that the Hilbert–Schmidt norm of an operator is equal to the norm of its integral kernel, Plancherel's formula, and Fubini's theorem, we have

$$\begin{aligned}\|H_u(h)\|^2_{HS}&=\frac{1}{16\pi^4}\left\|\int_0^\infty\!\!\int_0^\infty e^{ix\xi}e^{iy\eta}\hat{u}(\xi+\eta)\,d\eta\,d\xi\right\|^2_{L^2_{x,y}}=\frac{1}{4\pi^2}\|\mathbf{1}_{\xi\geq 0}\mathbf{1}_{\eta\geq 0}\hat{u}(\xi+\eta)\|^2_{L^2_{\eta,\xi}}\\ &=\frac{1}{4\pi^2}\int_0^\infty\!\!\int_0^\infty|\hat{u}(\xi+\eta)|^2\,d\eta\,d\xi=\frac{1}{4\pi^2}\int_0^\infty\!\!\int_\xi^\infty|\hat{u}(\zeta)|^2\,d\zeta\,d\xi\\ &=\frac{1}{4\pi^2}\int_0^\infty\left(\int_0^\zeta d\xi\right)|\hat{u}(\zeta)|^2\,d\zeta=\frac{1}{4\pi^2}\int_0^\infty\zeta|\hat{u}(\zeta)|^2\,d\zeta=\frac{1}{2\pi}\|u\|^2_{\dot{H}^{1/2}}.\end{aligned}$$

□

Lemma 3.6. Ker $H_u^2 = \operatorname{Ker} H_u$. *Moreover, if* Ran H_u *is finite-dimensional, then* Ran $H_u^2 = \operatorname{Ran} H_u$.

Proof. Let $f \in \operatorname{Ker} H_u^2$. Then, by (1-7) and the fact that $(H_u(h_1), h_2) = (H_u(h_2), h_1)$ for all $h_1, h_2 \in L^2_+$, we have

$$\|H_u f\|_{L^2}^2 = (H_u f, H_u f) = (H_u^2 f, f) = 0,$$

and thus $H_u f = 0$. Hence, Ker $H_u^2 \subset \operatorname{Ker} H_u$. Therefore, we obtain Ker $H_u^2 = \operatorname{Ker} H_u$ since the inverse inclusion is obvious.

The identity (1-7) yields also Ker $H_u = (\operatorname{Ran} H_u)^\perp$. Moreover, it implies that H_u^2 is a self-adjoint operator and therefore, Ker $H_u^2 = (\operatorname{Ran} H_u^2)^\perp$. Hence, we obtain

$$(\operatorname{Ran} H_u^2)^\perp = (\operatorname{Ran} H_u)^\perp.$$

Taking the orthogonal complement of both sides, this yields

$$\overline{\operatorname{Ran} H_u^2} = \overline{\operatorname{Ran} H_u}.$$

If Ran H_u is finite-dimensional, so is Ran H_u^2, since Ran $H_u^2 \subset \operatorname{Ran} H_u$. Thus, Ran H_u^2 and Ran H_u are closed. It follows that Ran $H_u^2 = \operatorname{Ran} H_u$. □

Lemma 3.7. *If u is a traveling wave, then*

$$A_u H_u^2 = H_u^2 A_u. \tag{3-3}$$

Consequently, if Ran H_u *is finite-dimensional, then* $A_u(\operatorname{Ran} H_u) \subset \operatorname{Ran} H_u$.

Proof. The commutativity relation (3-3) is a consequence of identity (1-10). The second statement then follows by Lemma 3.6, Ran $H_u^2 = \operatorname{Ran} H_u$. □

It is a classical fact that if A and B are two self-adjoint operators on a Hilbert space $\mathscr{H}$ such that $AB = BA$, then $B(\mathscr{H}_{\text{ac}}(A)) \subset \mathscr{H}_{\text{ac}}(A)$. For completeness, we prove this here in the case of A_u and H_u^2:

Lemma 3.8.
$$H_u^2 \mathscr{H}_{\text{ac}}(A_u) \subset \mathscr{H}_{\text{ac}}(A_u).$$

Proof. As we will see below, the inclusion follows if we prove that $\mu_{H_u^2\phi} \ll \mu_\phi$ for all $\phi \in L^2_+$, where the $\mu_{H_u^2\phi}$ and μ_ϕ denote the spectral measures of $H_u^2\phi$ and ϕ with respect to the operator A_u.

Let $E \subset \mathbb{R}$ be a measurable set and $f = \mathbf{1}_E$. By (3-3) and the Cauchy–Schwarz inequality we have

$$\begin{aligned}\mu_{H_u^2\phi}(E) &= \int_{\mathbb{R}} f \, d\mu_{H_u^2\phi} = (H_u^2\phi, f(A_u)H_u^2\phi) = (H_u^2\phi, H_u^2 f(A_u)\phi) = (H_u^4\phi, f(A_u)\phi) \\ &\le \sqrt{(f(A_u)\phi, f(A_u)\phi)}\|H_u^4\phi\|_{L^2} = \sqrt{(\phi, f(A_u)\phi)}\|H_u^4\phi\|_{L^2} = \sqrt{\mu_\phi(E)}\|H_u^4\phi\|_{L^2}.\end{aligned}$$

Therefore, $\mu_{H_u^2\phi} \ll \mu_\phi$. Denote by m the Lebesgue measure on $\mathbb{R}$. If $\phi \in \mathscr{H}_{\text{ac}}(A_u)$, then $\mu_\phi \ll m$ and thus $\mu_{H_u^2\phi} \ll m$. Hence, $H_u^2 \mathscr{H}_{\text{ac}}(A_u) \subset \mathscr{H}_{\text{ac}}(A_u)$. □

Proposition 3.9. *If u is a traveling wave, then* $\mathscr{H}_{\text{ac}}(A_u) \subset \operatorname{Ker} H_u$.

Proof. It is enough to prove that $[\Omega^+(D, A_u)H_u^2](\mathscr{H}_{\text{ac}}(A_u)) = 0$. If this holds, then $H_u^2(\mathscr{H}_{\text{ac}}(A_u)) = 0$ since $H_u^2\mathscr{H}_{\text{ac}}(A_u) \subset \mathscr{H}_{\text{ac}}(A_u)$ and $\Omega^+(D, A_u)$ is an isometry on $\mathscr{H}_{\text{ac}}(A_u)$. Therefore, $\mathscr{H}_{\text{ac}}(A_u) \subset$ Ker $H_u^2 = \operatorname{Ker} H_u$.

First note that

$$H_u e^{itD} = e^{itD} H_{\tau_t(u)}, \tag{3-4}$$

where τ_a denotes the translation $\tau_a u(x) = u(x-a)$. Indeed, for $f \in L^2_+$, passing into Fourier space, we have

$$\begin{aligned}\big(H_u e^{itD} f\big)^\wedge(\xi) &= \mathbf{1}_{\xi\geq 0}\big(u\overline{e^{itD} f}\big)^\wedge(\xi) = \frac{1}{2\pi}\mathbf{1}_{\xi\geq 0}\int_{\mathbb{R}} \hat{u}(\xi-\eta)e^{it\eta}\hat{\bar{f}}(\eta)\,d\eta \\ &= \frac{1}{2\pi}\mathbf{1}_{\xi\geq 0}e^{it\xi}\int e^{-it(\xi-\eta)}\hat{u}(\xi-\eta)\hat{\bar{f}}(\eta)\,d\eta = \mathbf{1}_{\xi\geq 0}e^{it\xi}\big(\tau_t(u)\bar{f}\,\big)^\wedge(\xi) \\ &= \mathbf{1}_{\xi\geq 0}\big(e^{itD}(\tau_t(u)\bar{f})\big)^\wedge(\xi) = \big(e^{itD}H_{\tau_t(u)}f\big)^\wedge(\xi).\end{aligned}$$

By Lemma 3.8, (3-3), and (3-4), we have for all $f \in \mathscr{H}_{\mathrm{ac}}(A_u)$

$$\begin{aligned}e^{itD}e^{-itA_u}P_{\mathrm{ac}}H_u^2 f &= e^{itD}e^{-itA_u}H_u^2 f = e^{itD}H_u^2 e^{-itA_u} f = e^{itD}H_u H_u e^{-itD}e^{itD}e^{-itA_u} f \\ &= e^{itD}H_u e^{-itD}H_{\tau_{-t}(u)}e^{itD}e^{-itA_u} f = H^2_{\tau_{-t}(u)}e^{itD}e^{-itA_u}P_{\mathrm{ac}}(A_u) f.\end{aligned}$$

We intend to prove that $H^2_{\tau_{-t}(u)}e^{itD}e^{-itA_u}P_{\mathrm{ac}}(A_u)f$ tends to 0 in the L^2_+-norm as $t\to-\infty$. From this, we conclude that $\Omega^+(D,A_u)H_u^2 f = 0$. Since, by Lemma 3.5, $H_{\tau_{-t}(u)}$ is uniformly bounded, it suffices to prove that $H_{\tau_{-t}(u)}e^{itD}e^{-itA_u}P_{\mathrm{ac}}(A_u)f$ tends to 0. We have

$$\begin{aligned}&\big\|H_{\tau_{-t}(u)}e^{itD}e^{-itA_u}P_{\mathrm{ac}}(A_u)f\big\|_{L^2_+} \\ &\quad\leq \big\|H_{\tau_{-t}(u)}\big(e^{itD}e^{-itA_u}P_{\mathrm{ac}}(A_u)f - \Omega^+(D,A_u)f\big)\big\|_{L^2_+} + \|H_{\tau_{-t}(u)}\Omega^+(D,A_u)f\|_{L^2_+} \\ &\quad\leq \frac{1}{\sqrt{2\pi}}\|u\|_{\dot{H}^{1/2}}\big\|e^{itD}e^{-itA_u}P_{\mathrm{ac}}(A_u)f - \Omega^+(D,A_u)f\big\|_{L^2_+} + \int_{\mathbb{R}}|u(x+t)|^2|\Omega^+(D,A_u)f(x)|^2\,dx\end{aligned} \tag{3-5}$$

The first term on the last line converges to 0 by the definition of the wave operator $\Omega^+(D,A_u)$. Since u is a traveling wave, we can write

$$u \in \bigcap_{s\geq 0} H^s(\mathbb{R}) \subset C^\infty_{\to 0}(\mathbb{R}),$$

where $C^\infty_{\to 0}(\mathbb{R})$ is the space of functions f of class C^∞ such that $\lim_{x\to-\infty} D^k f(x) = \lim_{x\to\infty} D^k f(x) = 0$ for all $k\in\mathbb{N}$. Therefore, for arbitrary fixed x, we have

$$\lim_{t\to-\infty}\tau_{-t}(u)(x) = \lim_{t\to-\infty} u(x+t) = 0.$$

Note also that

$$|u(x+t)|^2\,|\Omega^+(D,A_u)f(x)|^2 \leq \|u\|^2_{L^\infty}|\Omega^+(D,A_u)f(x)|^2$$

for all $x\in\mathbb{R}$. Thus the last term in (3-5) converges to 0 by the dominated convergence theorem. This shows that $\big[\Omega^+(D,A_u)H_u^2\big](\mathscr{H}_{\mathrm{ac}}(A_u)) = 0$. □

4. Classification of traveling waves

Lemma 4.1. *There are no nontrivial traveling waves of velocity $c = 0$ in $L^2_+(\mathbb{R})$.*

Proof. Let u be a nontrivial traveling wave of velocity $c = 0$. Then, (1-4) gives $\Pi(|u|^2 u) = \omega u$. Taking the scalar product with $e^{i\xi x}u(x)$, where $\xi \geq 0$, we obtain

$$\mathcal{F}(|u|^4 - \omega|u|^2)(\xi) = 0,$$

where $\mathcal{F}$ denotes the Fourier transform. Since $|u|^4 - \omega|u|^2$ is a real-valued function, we have that the last equality holds for all $\xi \in \mathbb{R}$. Thus $|u|^4 - \omega|u|^2 = 0$ on $\mathbb{R}$ and therefore $u(x) = 0$ or $|u(x)|^2 = \omega > 0$, for all $x \in \mathbb{R}$. Since the function u is holomorphic on $\mathbb{C}_+$, its trace on $\mathbb{R}$ is either identically zero, or the set of zeros of u on $\mathbb{R}$ has Lebesgue measure zero. In conclusion, we have $|u|^2 = \omega > 0$ a.e. on $\mathbb{R}$ and thus u is not a function in $L^2_+(\mathbb{R})$. □

Lemma 4.2. *If $u \in H^s_+$ for $s > \frac{1}{2}$ and $v \in \operatorname{Ker} H_u$, then $\bar{u}v \in L^2_+$. Moreover, if $u \in L^\infty(\mathbb{R})$, then $T_{|u|^2}v = |u|^2 v$.*

Proof. Indeed, $0 = H_u(v) = \Pi(u\bar{v})$ and thus $\bar{u}v \in L^2_+$. Furthermore, since $u, \bar{u}v \in L^2_+$, we obtain $T_{|u|^2}v = \Pi(u\bar{u}v) = |u|^2 v$. □

Lemma 4.3. *Let $u \in H^s_+$, $s > \frac{1}{2}$, be a solution of the cubic Szegő equation* (1-2). *For the Cauchy problem*

$$\begin{cases} i\partial_t \psi = |u(t)|^2 \psi \\ \psi|_{t=0} = \psi_0, \end{cases} \tag{4-1}$$

if $\psi_0 \in \operatorname{Ker} H_{u(0)}$, then $\psi(t) \in \operatorname{Ker} H_{u(t)}$ for all $t \in \mathbb{R}$.

Proof. Let us first consider

$$\begin{cases} i\partial_t \psi_1 = T_{|u(t)|^2}\psi_1 \\ \psi_1|_{t=0} = \psi_0, \end{cases}$$

Using the Lax pair structure, we have

$$\begin{aligned} \partial_t H_u(\psi_1) &= [B_u, H_u]\psi_1 + H_u \partial_t \psi_1 = \left[\tfrac{i}{2}H_u^2 - iT_{|u|^2}, H_u\right]\psi_1 + H_u(-iT_{|u|^2}\psi_1) \\ &= -iT_{|u|^2}H_u\psi_1 - iH_u T_{|u|^2}\psi_1 + iH_u T_{|u|^2}\psi_1 = -iT_{|u|^2}H_u\psi_1. \end{aligned}$$

The solution of the linear Cauchy problem

$$\begin{cases} \partial_t H_u(\psi_1) = -iT_{|u|^2}H_u\psi_1, \\ H_u(\psi_1(0)) = 0 \end{cases}$$

is identically zero: $H_{u(t)}\psi_1(t) = 0$ for all $t \in \mathbb{R}$. Consequently, $\psi_1(t) \in \operatorname{Ker} H_{u(t)}$, and by Lemma 4.2 we obtain $T_{|u|^2}\psi_1 = |u|^2\psi_1$. In conclusion, $\psi(t) = \psi_1(t) \in \operatorname{Ker} H_{u(t)}$. □

The space $\operatorname{Ker} H_u$ is invariant under multiplication by $e^{i\alpha x}$, for all $\alpha \geq 0$. Indeed, suppose $f \in \operatorname{Ker} H_u$. Then $(u\bar{f})^\wedge(\xi) = 0$, for all $\xi \geq 0$ and

$$\big(H_u(e^{i\alpha x}f)\big)^\wedge(\xi) = \big(e^{-i\alpha x}u\bar{f}\big)^\wedge(\xi) = (u\bar{f})^\wedge(\xi + \alpha) = 0,$$

for all $\xi, \alpha \geq 0$. Hence, $e^{i\alpha x}f \in \operatorname{Ker} H_u$ for all $\alpha \geq 0$.

One can then apply the following theorem to the subspaces $\operatorname{Ker} H_{u_0}$.

Proposition 4.4 [Lax 1959]. *Every nonempty closed subspace of L^2_+ that is invariant under multiplication by $e^{i\alpha x}$ for all $\alpha \geq 0$ is of the form FL^2_+, where F is an analytic function in the upper-half plane, $|F(z)| \leq 1$ for all $z \in \mathbb{C}_+$, and $|F(x)| = 1$ for all $x \in \mathbb{R}$. Moreover, F is uniquely determined up to multiplication by a complex constant of absolute value* 1.

We deduce that $\operatorname{Ker} H_{u_0} = \phi L^2_+$, where ϕ is a holomorphic function in the upper half-plane $\mathbb{C}_+$, satisfying $|\phi(x)| = 1$ on $\mathbb{R}$ and $|\phi(z)| \leq 1$ for all $z \in \mathbb{C}_+$.

Functions satisfying the properties in Proposition 4.4 are called inner functions in the sense of Beurling and Lax. A special class of such functions is that of Blaschke products. Given $\lambda_j \in \mathbb{C}$ such that for all j

$$\operatorname{Im} \lambda_j > 0 \quad \text{and} \quad \sum_j \frac{\operatorname{Im} \lambda_j}{1 + |\lambda_j|^2} < \infty,$$

the corresponding Blaschke product is defined by

$$B(z) = \prod_j \varepsilon_j \frac{z - \lambda_j}{z - \bar{\lambda}_j}, \quad \text{where } \varepsilon_j = \frac{|\lambda_j^2+1|}{\lambda_j^2+1} \tag{4-2}$$

(by definition $\varepsilon_j = 1$ if $\lambda_j = 1$).

Inner functions have a canonical factorization, which is analogous to the canonical factorization of inner functions on the unit disk; see [Rudin 1974, Theorem 17.15] or [Nikolski 2002, Theorem 6.4.4]. More precisely, every inner function F can be written as the product

$$F(z) = \lambda B(z) e^{iaz} \exp\left(i \int_{\mathbb{R}} \frac{1 + tz}{t - z} \, d\nu(t) \right), \tag{4-3}$$

where $z \in \mathbb{C}_+$, $\lambda \in \mathbb{C}$ with $|\lambda| = 1$, $a \geq 0$, B is a Blaschke product, and ν is a positive singular measure with respect to the Lebesgue measure. In particular, the inner function ϕ has such a canonical factorization.

Proposition 4.5. *Let u be a traveling wave and denote by ϕ an inner function such that* $\operatorname{Ker} H_{u_0} = \phi L^2_+$. *Then, ϕ satisfies the following equation on* $\mathbb{R}$:

$$cD\phi = |u_0|^2 \phi. \tag{4-4}$$

Proof. Since $u(t, x) = e^{-i\omega t} u_0(x - ct)$, we have $H_{u(t)} = e^{-i\omega t} \tau_{ct} H_{u_0} \tau_{-ct}$. Thus,

$$\operatorname{Ker} H_{u(t)} = \tau_{ct} \operatorname{Ker} H_{u_0} = \tau_{ct}(\phi) L^2_+.$$

Let $f \in L^2_+$ and let $\psi_0 = \phi f \in \operatorname{Ker} H_{u_0}$ be the initial data of the Cauchy problem (4-1) in Lemma 4.3. We then have $\phi e^{-i \int_0^t |u(s)|^2 \, ds} f \in \operatorname{Ker} H_{u(t)}$. Therefore,

$$\phi e^{-i \int_0^t |u(s)|^2 \, ds} L^2_+ \subset \tau_{ct}(\phi) L^2_+. \tag{4-5}$$

Conversely, by solving backward the problem (4-1) with the initial data in $\tau_{ct}(\phi) L^2_+$ at time t, up to the time $t = 0$, we obtain

$$\tau_{ct}(\phi) L^2_+ \subset \phi e^{-i \int_0^t |u(s)|^2 \, ds} L^2_+$$

and thus, the two sets are equal.

Let us first prove that $\phi_t := \phi e^{-i\int_0^t |u(s)|^2\,ds}$ is an inner function. Note that ϕ_t is well defined on $\mathbb{R}$ and its absolute value is 1 on $\mathbb{R}$. Consider the function defined by $h(x) = \phi_t(x)/(x+i)$ for $x \in \mathbb{R}$. Since $h \in L^2_+$, we can write using the Poisson integral that

$$h(z) = \frac{1}{\pi}\int_{-\infty}^{\infty} \operatorname{Im} z \frac{h(x)}{|z-x|^2}\,dx$$

for all $z \in \mathbb{C}_+$. Then,

$$zh(z) = \frac{1}{\pi}\int_{-\infty}^{\infty} \operatorname{Im} z \frac{xh(x)}{|z-x|^2}\,dx + \frac{1}{\pi}\int_{-\infty}^{\infty} \operatorname{Im} z \frac{(z-x)h(x)}{|z-x|^2}\,dx.$$

Note that the last integral is equal to

$$\int_{-\infty}^{\infty} \operatorname{Im} z \frac{h(x)}{\bar{z}-x}\,dx.$$

By the residue theorem and using the fact that the function $h/(\bar{z}-x)$ is holomorphic on $\mathbb{C}_+$, we have that this integral is zero and thus

$$zh(z) = \frac{1}{\pi}\int_{-\infty}^{\infty} \operatorname{Im} z \frac{xh(x)}{|z-x|^2}\,dx.$$

Therefore, we can use the Poisson integral to extend ϕ_t to $\mathbb{C}_+$ as a holomorphic function.

$$\phi_t(z) = (z+i)h(z) = \frac{1}{\pi}\int_{-\infty}^{\infty} \operatorname{Im} z \frac{(x+i)h(x)}{|z-x|^2}\,dx = \frac{1}{\pi}\int_{-\infty}^{\infty} \operatorname{Im} z \frac{\phi_t(x)}{|z-x|^2}\,dx. \tag{4-6}$$

Moreover,

$$|\phi_t(z)| \le \frac{1}{\pi}\int_{-\infty}^{\infty} \operatorname{Im} z \frac{1}{|z-x|^2}\,dx = 1,$$

for all $z \in \mathbb{C}_+$. Hence ϕ_t is an inner function.

Since $\tau_{ct}(\phi)$ and $\phi e^{-i\int_0^t |u(s)|^2\,ds}$ are inner functions and

$$\phi e^{-i\int_0^t |u(s)|^2\,ds} L^2_+ = \tau_{ct}(\phi) L^2_+,$$

Proposition 4.4 yields the existence of a real-valued function γ such that $\gamma(0) = 0$ and

$$\phi e^{-i\int_0^t |u(s)|^2\,ds} = \tau_{ct}(\phi) e^{i\gamma(t)}.$$

Taking the derivative with respect to t, we obtain that ϕ satisfies the equation

$$cD\phi(x) = |u(t, x+ct)|^2\phi(x) + \dot{\gamma}(t)\phi(x).$$

for all $t \in \mathbb{R}$. Since u is a traveling wave, we have $|u(t, x+ct)| = |e^{-i\omega t}u_0(x)| = |u_0(x)|$. Then we deduce that $\dot{\gamma}(t) = k$ and hence $\gamma(t) = kt$, for some $k \in \mathbb{R}$. Therefore,

$$cD\phi = (|u_0|^2 + k)\phi. \tag{4-7}$$

We prove in the following that $k = 0$. First, note that $\frac{k}{c} \geq 0$. The function $\phi u_0 \in \operatorname{Ker} H_{u_0}$ and by Lemma 4.2, we have $|u_0|^2\phi = \overline{u}_0(u_0\phi) \in L^2_+$. If k/c is negative, setting $\chi := \frac{1}{c}|u_0|^2\phi \in L^2_+$ and passing into Fourier space, we have

$$\hat{\phi}(\xi) = \frac{1}{\xi - k/c}\hat{\chi}(\xi)\, \mathbf{1}_{[0,\infty)}(\xi).$$

This implies that $\phi \in L^2_+$, contradicting $|\phi(x)| = 1$ for all $x \in \mathbb{R}$.

Let us now prove that $k/c = 0$. Let $h \in L^2_+$ be regular. Then $\phi h \in \operatorname{Ker} H_{u_0}$, and by (4-7) we have

$$A_{u_0}(\phi h) = \Big(D - \frac{1}{c}|u_0|^2\Big)(\phi h) = \phi\Big(D - \frac{1}{c}|u_0|^2\Big)(h) + hD\phi = \phi\Big(D + \frac{k}{c}\Big)h.$$

Denoting by $\mu_{\phi h}(A_{u_0})$ the spectral measure corresponding to ϕh, we have

$$\begin{aligned}\int f d\mu_{\phi h} &= (\phi h, f(A_{u_0})\phi h) = \Big(\phi h, \phi f\Big(D + \frac{k}{c}\Big)h\Big) = \Big(h, f\Big(D + \frac{k}{c}\Big)h\Big) \\ &= \frac{1}{2\pi}\int_0^\infty f\Big(\xi + \frac{k}{c}\Big)|\hat{h}(\xi)|^2\, d\xi = \frac{1}{2\pi}\int_{k/c}^\infty f(\eta)\Big|\hat{h}\Big(\eta - \frac{k}{c}\Big)\Big|^2 d\eta.\end{aligned}$$

Consequently, $\operatorname{supp}\mu_{\phi h}(A_{u_0}) \subset [k/c, +\infty)$. By Proposition 3.9, we have $\mathcal{H}_{\mathrm{ac}}(A_{u_0}) \subset \operatorname{Ker} H_{u_0}$, and therefore

$$\sigma_{\mathrm{ac}}(A_{u_0}) = \overline{\bigcup_{\psi \in \mathcal{H}_{\mathrm{ac}}(A_{u_0})} \operatorname{supp}\mu_\psi} \subset \overline{\bigcup_{\phi h \in \operatorname{Ker} H_{u_0}} \operatorname{supp}\mu_{\phi h}} \subset \Big[\frac{k}{c}, \infty\Big).$$

Since, by Corollary 3.4, $\sigma_{\mathrm{ac}}(A_{u_0}) = [0, \infty)$, this yields $k = 0$. □

Proposition 4.6. *All traveling waves are rational functions.*

Proof. We first prove that ϕ is a Blaschke product.

Since ϕ is an inner function in the sense of Beurling and Lax, it has the canonical decomposition

$$\phi(z) = \lambda B(z)e^{iaz}\exp\Big(i\int_{\mathbb{R}} \frac{1 + tz}{t - z}\, d\nu(t)\Big), \tag{4-8}$$

where $z \in \mathbb{C}_+$, λ is a complex number of absolute value 1, $a \geq 0$, B is a Blaschke product having exactly the same zeroes as ϕ, and ν is a positive singular measure with respect to the Lebesgue measure.

Because ϕ satisfies (4-4) and $u_0 \in L^\infty(\mathbb{R})$, we obtain that ϕ has bounded derivative on $\mathbb{R}$ and hence it is uniformly continuous on $\mathbb{R}$. Then, since ϕ satisfies the Poisson formula (4-6), it follows that

$$\phi(x + i\varepsilon) \to \phi(x), \text{ as } \varepsilon \to 0,$$

uniformly for $x \in \mathbb{R}$. Since ϕ is uniformly continuous on $\mathbb{R}$ and since $|\phi(x)| = 1$ for all $x \in \mathbb{R}$, we deduce that the zeroes of ϕ, and hence those of the Blaschke product B as well, lie outside a strip $\{z \in \mathbb{C}; 0 \leq \operatorname{Im} z \leq \varepsilon_0\}$, for some $\varepsilon_0 > 0$. Therefore, we have

$$\frac{\phi(x + i\varepsilon)}{B(x + i\varepsilon)} \to \frac{\phi(x)}{B(x)} \quad \text{as } \varepsilon \to 0$$

uniformly for x in compact subsets of $\mathbb{R}$. Taking the logarithm of the absolute value and noticing that $|\phi(x)/B(x)| = 1$, we obtain

$$\int_{\mathbb{R}} \frac{\varepsilon}{(x-t)^2+\varepsilon^2}\, d\nu(t) \to 0,$$

uniformly for x in compact subsets in $\mathbb{R}$. In particular, for all $\delta > 0$ there exists $0 < \varepsilon_1 \le \varepsilon_0$ such that for all $0 < \varepsilon \le \varepsilon_1$ and for all $x \in [0, 1]$, we have

$$\frac{1}{2\varepsilon}\nu([x-\varepsilon, x+\varepsilon]) \le \int_{x-\varepsilon}^{x+\varepsilon} \frac{\varepsilon}{(x-t)^2+\varepsilon^2}\, d\nu(t) \le \int_{\mathbb{R}} \frac{\varepsilon}{(x-t)^2+\varepsilon^2}\, d\nu(t) \le \delta.$$

Taking $\varepsilon = \dfrac{1}{2N} \le \varepsilon_1$ with $N \in \mathbb{N}^*$, we obtain

$$\nu([0,1]) = \nu\biggl(\bigcup_{k=0}^{N-1}\Bigl[\frac{k}{N}, \frac{k+1}{N}\Bigr]\biggr) \le N\delta\frac{1}{N} = \delta.$$

In conclusion, $\nu([0, 1]) = 0$, and one can prove similarly that the measure ν of any compact interval in $\mathbb{R}$ is zero. Hence $\nu \equiv 0$.

Consequently, $\phi(x) = \lambda B(x)e^{iax}$ for all $x \in \mathbb{R}$. On the other hand, because ϕ satisfies (4-4), we have $\phi(x) = \phi(0)e^{(i/c)\int_0^x |u_0|^2}$ and, in particular, $\lim_{x\to\infty} \phi(x) = \phi(0)e^{(i/c)\int_0^\infty |u_0|^2}$. Since $\lim_{x\to\infty} B(x) = 1$, we conclude that $a = 0$. Substituting $\phi = \lambda B$ (4-4), we obtain

$$\frac{c}{i}\frac{B'}{B} = |u_0|^2.$$

Then

$$\frac{1}{i}\int_{-\infty}^{\infty} \frac{B'(x)}{B(x)}\, dx < \infty.$$

Computing this integral, we obtain that

$$\frac{1}{i}\int_{-\infty}^{\infty} \frac{B'(x)}{B(x)}\, dx = 2\sum_j \int_{-\infty}^{\infty} \frac{\operatorname{Im}\lambda_j}{|x-\lambda_j|^2}\, dx = 2\sum_j \pi$$

and thus it is finite if and only if B is a finite Blaschke product, $B(x) = \prod_{j=1}^N \varepsilon_j \dfrac{x-\lambda_j}{x-\bar{\lambda}_j}$.

We prove that the traveling wave u is a rational function. We have

$$\operatorname{Ker} H_u = \phi L^2_+ = BL^2_+.$$

Set $Y := \operatorname{span}_{\mathbb{C}}\Bigl\{\dfrac{1}{x-\bar{\lambda}_j}\Bigr\}_{j=1}^N$; we show that $BL^2_+ = Y^\perp$. Indeed, $f \in Y^\perp$ if and only if

$$f(\lambda_j) = \frac{1}{2\pi}\int_{\mathbb{R}} e^{i\xi\lambda_j}\,\widehat{f}(\xi)\, d\xi = \frac{1}{2\pi}\bigl(\hat{f}, e^{-i\bar{\lambda}_j\xi}\bigr) = \Bigl(f, \frac{1}{x-\bar{\lambda}_j}\Bigr) = 0,$$

if and only if there exists $h \in L^2_+$ such that $f = Bh$. Hence $\operatorname{Ker} H_u = Y^\perp$. This yields $\overline{\operatorname{Ran} H_u} = Y$. By Remark 2.2 it follows that u is a rational function. More precisely, $u \in \operatorname{Ran} H_u = Y$. ☐

Proposition 4.7. *If u is a traveling wave, there exists $\lambda > 0$ such that $H_u^2 u = \lambda u$.*

Proof. According to Remark 2.2, since u is a rational function, we have $u \in \operatorname{Ran} H_u$.

Secondly, u satisfies the equation of the traveling waves (1-4), which is equivalent to $A_u(u) = -\frac{\omega}{c}u$. Therefore, u is an eigenfunction of the operator A_u for the eigenvalue $-\omega/c$. Applying the identity (1-10),

$$A_u H_u + H_u A_u + \frac{\omega}{c} H_u + \frac{1}{c} H_u^3 = 0,$$

to u and then to $H_u u$, one deduces that $A_u H_u^2 u = -\frac{\omega}{c} H_u^2 u$. Therefore, the conclusion of the proposition follows once we prove all the eigenfunctions of the operator A_u belonging to Ran H_u, corresponding to the same eigenvalue, are linearly dependent.

Let a be en eigenvalue of the operator A_u and let $\psi_1, \psi_2 \in \operatorname{Ker}(A_u - a) \cap \operatorname{Ran} H_u$. Since u is a rational function, by the Kronecker type Theorem 2.1, ψ_1 and ψ_2 are also nonconstant rational functions. Then, one can find $\alpha, \beta \in \mathbb{C}$, $(\alpha, \beta) \neq (0,0)$, such that $\psi := \alpha\psi_1 + \beta\psi_2 = O(\frac{1}{x^2})$ as $x \to \infty$. Moreover, we have $\psi \in L^1(\mathbb{R})$, $x\psi \in L^2(\mathbb{R})$, and thus we can compute $A_u(x\psi)$.

Passing into Fourier space we have

$$\widehat{\Pi(xf)}(\xi) = i(\partial_\xi \hat{f})\mathbf{1}_{\xi\geq 0} = i\partial_\xi(\hat{f}\mathbf{1}_{\xi\geq 0}) - i\hat{f}(\xi)\delta_{\xi=0} = \widehat{x\Pi f}(\xi) - i\hat{f}(0)\delta_{\xi=0},$$

for all $f \in L^1(\mathbb{R})$. Thus, we obtain $\Pi(xf) = x\Pi(f) + \frac{1}{2\pi i}\hat{f}(0)$ for all $f \in L^1(\mathbb{R})$. We then have

$$A_u(x\psi) = xA_u(\psi) + \frac{1}{i}\psi - \frac{1}{2c\pi i}\int_{\mathbb{R}} |u|^2\psi\, dx$$

and therefore, since $A_u\psi = a\psi$,

$$A_u(x\psi) = ax\psi + \frac{1}{i}\psi - \frac{1}{2c\pi i}\int_{\mathbb{R}} |u|^2\psi\, dx. \tag{4-9}$$

Since $x\psi \in \operatorname{Ran} H_u$ and $A_u(\operatorname{Ran} H_u) \subset \operatorname{Ran} H_u$ by Lemma 3.7, we have $A_u(x\psi) \in \operatorname{Ran} H_u \subset L^2(\mathbb{R})$. The constant in (4-9) is zero because all the other terms are in $L^2(\mathbb{R})$. Then we have

$$(A_u - a)(x\psi) = \frac{1}{i}\psi. \tag{4-10}$$

Applying the self-adjoint operator $A_u - a$ to both sides of (4-10), we obtain $(A_u - a)^2(x\psi) = 0$ and

$$\|(A_u - a)(x\psi)\|_{L^2}^2 = \big((A_u - a)(x\psi), (A_u - a)(x\psi)\big) = \big((A_u - a)^2(x\psi), x\psi\big) = 0.$$

Thus, $(A_u - a)(x\psi) = 0$. In conclusion, by (4-10), $\psi = 0$ and therefore all the eigenfunctions belonging to Ran H_u, corresponding to the same eigenvalue a, are linearly dependent. □

Proof of Theorem 1.2. Since $u \in \operatorname{Ran} H_u$, there exists a unique function $g \in \operatorname{Ran} H_u$ such that $u = H_u(g)$. By Proposition 4.7, it results that $H_u(u) = \lambda g$. Applying the identity (1-10),

$$A_u H_u + H_u A_u + \frac{\omega}{c} H_u + \frac{1}{c} H_u^3 = 0,$$

to g and using $A_u u = -\dfrac{\omega}{c}u$, one obtains

$$H_u\Big(A_u g + \frac{\lambda}{c} g\Big) = 0.$$

Since $A_u(\mathrm{Ran}\, H_u) \subset \mathrm{Ran}\, H_u$, we have

$$A_u g + \frac{\lambda}{c} g \in \mathrm{Ran}\, H_u \cap \mathrm{Ker}\, H_u.$$

Therefore, $A_u g + \frac{\lambda}{c} g = 0$, which is equivalent to

$$cDg - T_{|u|^2} g + \lambda g = 0.$$

We next find a simpler version of this equation, in order to determine the function g explicitly. Note that $\bar{u}(1-g) \in L^2_+$, since it is orthogonal to each complex conjugate of a holomorphic function $f \in L^2_+$:

$$(\bar{u}(1-g), \bar{f}) = (f(1-g), u) = (f, u) - (f, H_u(g)) = 0.$$

Thus,

$$T_{|u|^2}(g) = \Pi(|u|^2) - \Pi(|u|^2(1-g)) = H_u(u) - |u|^2(1-g) = \lambda g - |u|^2(1-g).$$

Passing into Fourier space and using the fact that $|u|^2$ is a real-valued function, one can write

$$|u|^2 = \int_0^\infty e^{ix\xi} \widehat{|u|^2}(\xi)\, d\xi + \int_0^\infty e^{-ix\xi} \overline{\widehat{|u|^2}}(\xi)\, d\xi = \Pi(|u|^2) + \overline{\Pi(|u|^2)}.$$

Therefore $|u|^2 = H_u(u) + \overline{H_u(u)} = \lambda(g + \bar{g})$. Consequently, $T_{|u|^2}(g) = \lambda(-\bar{g} + g^2 + |g|^2)$ and g solves the equation

$$cDg - \lambda g^2 + \lambda(g + \bar{g} - |g|^2) = 0. \tag{4-11}$$

We prove that $g + \bar{g} - |g|^2 = 0$. First, note that $\bar{u}(1-g) \in L^2_+$, also yields $(1-g)f \in \mathrm{Ker}\, H_u$, for all $f \in L^2_+$. Secondly, let us prove that $g + \bar{g} - |g|^2$ is orthogonal to the complex conjugate of all $f \in L^2_+$:

$$(g + \bar{g} - |g|^2, \bar{f}) = (g, \bar{f}) - (f(1-g), g) = -\Big(f(1-g), \frac{1}{\lambda} H_u(u)\Big) = -\frac{1}{\lambda}\Big(u, H_u(f(1-g))\Big) = 0.$$

In addition, since $g + \bar{g} - |g|^2$ is a real-valued function, we have

$$(g + \bar{g} - |g|^2, f) = (g + \bar{g} - |g|^2, \bar{f}) = 0$$

for all $f \in L^2_+$. Therefore, $g+\bar{g}-|g|^2$ is orthogonal to all the functions in $L^2(\mathbb{R})$ and thus $g+\bar{g}-|g|^2 = 0$. This is equivalent to $|1-g| = 1$ on $\mathbb{R}$. Moreover, (4-11) gives the precise formula for g:

$$g(z) = \frac{r}{z-p},$$

where $r, p \in \mathbb{C}$ and $\mathrm{Im}(p) < 0$. Thus $1 - g(x) = \frac{x-\bar{p}}{x-p}$ for all $x \in \mathbb{R}$ and

$$\mathrm{Ker}\, H_{\frac{1}{z-p}} = \frac{z-\bar{p}}{z-p} L^2_+ = (1-g)L^2_+ \subset \mathrm{Ker}\, H_u.$$

Consequently, $u \in \mathrm{Ran}\, H_u \subset \mathrm{Ran}\, H_{\frac{1}{z-p}} = \frac{\mathbb{C}}{z-p}$. □

5. Orbital stability of traveling waves

In order to prove the orbital stability of traveling waves, we first use the fact that they are minimizers of the Gagliardo–Nirenberg inequality. We begin this section by proving this inequality:

Proof of Proposition 1.5, the Gagliardo–Nirenberg inequality. The proof is similar to that of the Gagliardo–Nirenberg inequality for the circle, in [Gérard and Grellier 2010b]. The idea is to write all the norms in the Fourier space, using Plancherel's identity.

$$E = \|u\|_{L^4}^4 = \|u^2\|_{L^2}^2 = \frac{1}{2\pi}\|\widehat{u^2}\|_{L^2}^2 = \frac{1}{2\pi}\int_{\mathbb{R}} |\widehat{u^2}(\xi)|^2\, d\xi.$$

Using the fact that $u \in L^2_+$ and Cauchy–Schwarz inequality, we have

$$\begin{aligned} |\widehat{u^2}(\xi)|^2 &= \frac{1}{4\pi^2}\left|\int_0^\xi \widehat{u}(\eta)\widehat{u}(\xi-\eta)\, d\eta\right|^2 \le \frac{1}{4\pi^2}\xi \int_0^\xi |\widehat{u}(\eta)|^2|\widehat{u}(\xi-\eta)|^2\, d\eta \\ &\le \frac{1}{4\pi^2}\left(\int_0^\xi \eta|\widehat{u}(\eta)|^2|\widehat{u}(\xi-\eta)|^2\, d\eta + \int_0^\xi (\xi-\eta)|\widehat{u}(\eta)|^2|\widehat{u}(\xi-\eta)|^2\, d\eta\right). \end{aligned}$$

By the change of variables $\xi-\eta \mapsto \eta$ in the second integral, we have

$$|\widehat{u^2}(\xi)|^2 \le \frac{1}{2\pi^2}\int_0^\xi \eta|\widehat{u}(\eta)|^2|\widehat{u}(\xi-\eta)|^2\, d\eta.$$

By Fubini's theorem and change of variables $\zeta = \xi-\eta$ it results that

$$E \le \frac{1}{4\pi^3}\int_{\mathbb{R}}\int_0^\xi \eta|\widehat{u}(\eta)|^2|\widehat{u}(\xi-\eta)|^2\, d\eta d\xi = \frac{1}{4\pi^3}\int_0^{+\infty}\eta|\widehat{u}(\eta)|^2\, d\eta \int_0^{+\infty}|\widehat{u}(\zeta)|^2\, d\zeta = \frac{1}{\pi}MQ.$$

Equality holds if and only if we have equality in Cauchy–Schwarz inequality, i.e.

$$\widehat{u}(\xi)\widehat{u}(\eta) = \widehat{u}(\xi+\eta)\widehat{u}(0),$$

for all $\xi, \eta \ge 0$. This is true if and only if

$$\widehat{u}(\xi) = e^{-ip\xi}\widehat{u}(0) \quad \text{for all } \xi \ge 0.$$

Since $u \in H^{1/2}_+$, this yields $\operatorname{Im}(p) < 0$ and $u(x) = C/(x-p)$, for some constant C. □

The second argument we use in proving the stability of traveling waves is a profile decomposition theorem. It states that bounded sequences in $H^{1/2}_+$ can be written as superposition of translations of fixed profiles and of a remainder term. The remainder is small in all the L^p-norms, $2 < p < \infty$. Moreover, the superposition is almost orthogonal in the $H^{1/2}_+$-norm.

Proposition 5.1 (Profile decomposition theorem for bounded sequences in $H^{1/2}_+$). *Let $\{v^n\}_{n\in\mathbb{N}}$ be a bounded sequence in $H^{1/2}_+$. There exist a subsequence of $\{v^n\}_{n\in\mathbb{N}}$, still denoted by $\{v^n\}_{n\in\mathbb{N}}$, a sequence of fixed profiles in $H^{1/2}_+$, $\{V^{(j)}\}_{j\in\mathbb{N}}$, and a family of real sequences $\{x^{(j)}\}_{j\in\mathbb{N}}$ such that for all $\ell \in \mathbb{N}^*$ we have*

$$v^n = \sum_{j=1}^{\ell} V^{(j)}(x - x_n^{(j)}) + r_n^{(\ell)},$$

where

$$\lim_{\ell\to\infty}\limsup_{n\to\infty}\|r_n^{(\ell)}\|_{L^p(\mathbb{R})}=0$$

for all $p\in(2,\infty)$, *and*

$$\|v^n\|_{L^2}^2=\sum_{j=1}^{\ell}\|V^{(j)}\|_{L^2}^2+\|r_n^{(\ell)}\|_{L^2}^2+o(1) \qquad \text{as } n\to\infty,$$

$$\|v^n\|_{\dot H_+^{1/2}}^2=\sum_{j=1}^{\ell}\|V^{(j)}\|_{\dot H_+^{1/2}}^2+\|r_n^{(\ell)}\|_{\dot H_+^{1/2}}^2+o(1) \quad \text{as } n\to\infty,$$

$$\lim_{n\to\infty}\|v^n\|_{L^4}^4=\sum_{j=1}^{\infty}\|V^{(j)}\|_{L^4}^4.$$

The proof of this proposition follows exactly the same lines as that of the profile decomposition theorem for bounded sequences in $H^1(\mathbb{R})$; see [Hmidi and Keraani 2006, Proposition 2.1]. However, note that in our case, the profiles $V^{(j)}$ belong to the space $H_+^{1/2}$ (not only to the space $H^{1/2}(\mathbb{R})$), as they are weak limits of translations of the sequence $\{v^n\}_{n\in\mathbb{N}}$.

Proof of Theorem 1.3. According to Proposition 1.5, $C(a,r)$ is the set of minimizers of the problem

$$\inf\bigl\{M(u);u\in H_+^{1/2},\ Q(u)=q(a,r),\ E(u)=e(a,r)\bigr\},$$

where

$$q(a,r)=\frac{a^2\pi}{r},\qquad e(a,r)=\frac{a^4\pi}{2r^3}.$$

We denote the infimum by $m(a,r)$. Since

$$\inf_{\phi\in C(a,r)}\|u_0^n-\phi\|_{H_+^{1/2}}\to 0,$$

by the Sobolev embedding theorem, we deduce

$$Q(u_0^n)\to q(a,r),\qquad E(u_0^n)\to e(a,r),\qquad M(u_0^n)\to m(a,r).$$

Let $\{t_n\}_{n\in\mathbb{N}}$ be an arbitrary sequence of real numbers. The conservation laws yield

$$Q(u^n(t_n))\to q(a,r),\quad E(u^n(t_n))\to e(a,r),\quad M(u^n(t_n))\to m(a,r).$$

We can choose two sequences of positive numbers $\{a_n\}$ and $\{\lambda_n\}$ such that $v^n(x):=a_nu^n(t_n,\lambda_nx)$ satisfies $\|v^n\|_{L^2(\mathbb{R})}=1$, $\|v^n\|_{L^4(\mathbb{R})}=1$. Notice that

$$a_n\to a_\infty,\quad \lambda_n\to\lambda_\infty,$$

where $a_\infty>0$, $\lambda_\infty>0$, and

$$\frac{\lambda_\infty}{a_\infty^4}=e(a,r),\quad \frac{\lambda_\infty}{a_\infty^2}=q(a,r).$$

Then

$$\|v^n\|_{\dot H^{1/2}_+}^{1/2} = \frac{\|v^n\|_{L^2}^{1/2}\|v^n\|_{\dot H^{1/2}_+}^{1/2}}{\|v^n\|_{L^4}} = \frac{\|u^n(t_n)\|_{L^2}^{1/2}\|u^n(t_n)\|_{\dot H^{1/2}_+}^{1/2}}{\|u^n(t_n)\|_{L^4}} \quad \text{for all } n \in \mathbb{N}.$$

In particular, as a consequence of the Gagliardo–Nirenberg inequality,

$$\lim_{n\to\infty} \|v^n\|_{\dot H^{1/2}_+} = \sqrt{\pi}.$$

Thus the sequence $\{v^n\}_{n\in\mathbb{N}}$ is bounded in $H^{1/2}_+$. From the profile decomposition theorem (Proposition 5.1), we obtain that there exist real sequences $\{x^{(j)}\}_{j\in\mathbb{N}}$ depending on the sequence $\{t_n\}_{n\in\mathbb{N}}$ in the definition of $\{v^n\}_{n\in\mathbb{N}}$, such that for all $\ell \in \mathbb{N}^*$ we have

$$v^n = \sum_{j=1}^{\ell} V^{(j)}(x - x_n^{(j)}) + r_n^{(\ell)},$$

where

$$\lim_{\ell\to\infty} \limsup_{n\to\infty} \|r_n^{(\ell)}\|_{L^p(\mathbb{R})} = 0$$

for all $p \in (2, \infty)$, and

$$\begin{aligned}
\|v^n\|_{L^2}^2 &= \sum_{j=1}^{\ell} \|V^{(j)}\|_{L^2}^2 + \|r_n^{(\ell)}\|_{L^2}^2 + o(1) && \text{as } n \to \infty,\\
\|v^n\|_{\dot H^{1/2}_+}^2 &= \sum_{j=1}^{\ell} \|V^{(j)}\|_{\dot H^{1/2}_+}^2 + \|r_n^{(\ell)}\|_{\dot H^{1/2}_+}^2 + o(1) && \text{as } n \to \infty,\\
\lim_{n\to\infty} \|v^n\|_{L^4}^4 &= \sum_{j=1}^{\infty} \|V^{(j)}\|_{L^4}^4.
\end{aligned}$$

Consequently,

$$1 \ge \sum_{j=1}^{\infty} \|V^{(j)}\|_{L^2}^2, \qquad \pi \ge \sum_{j=1}^{\infty} \|V^{(j)}\|_{\dot H^{1/2}_+}^2, \qquad 1 = \sum_{j=1}^{\infty} \|V^{(j)}\|_{L^4}^4. \tag{5-1}$$

Therefore, by the Gagliardo–Nirenberg inequality (1-12), we have

$$\pi \ge \Big(\sum_{j=1}^{\infty} \|V^{(j)}\|_{L^2}^2\Big)\Big(\sum_{j=1}^{\infty} \|V^{(j)}\|_{\dot H^{1/2}_+}^2\Big) \ge \sum_{j=1}^{\infty} \|V^{(j)}\|_{L^2}^2 \|V^{(j)}\|_{\dot H^{1/2}_+}^2 \ge \pi \sum_{j=1}^{\infty} \|V^{(j)}\|_{L^4}^4 = \pi.$$

Thus, there exist only one profile $V := V^{(1)}$ and a sequence $x = x^{(1)}$ such that

$$\begin{aligned}
v^n &= V(x - x_n) + r_n,\\
\|v^n\|_{L^2}^2 &= \|V\|_{L^2}^2 + \|r_n\|_{L^2}^2 + o(1) \qquad \text{as } n \to \infty, && (5\text{-}2)\\
\|v^n\|_{\dot H^{1/2}_+}^2 &= \|V\|_{\dot H^{1/2}_+}^2 + \|r_n\|_{\dot H^{1/2}_+}^2 + o(1) \qquad \text{as } n \to \infty. && (5\text{-}3)
\end{aligned}$$

According to (5-1), V satisfies $1 \geq \|V\|_{L^2}^2$, $\pi \geq \|V\|_{\dot{H}_+^{1/2}}^2$, and $\|V\|_{L^4}^4 = 1$. In conclusion,

$$\pi = \pi \|V\|_{L^4}^4 \leq \|V\|_{L^2}^2 \|V\|_{\dot{H}_+^{1/2}}^2 \leq \pi.$$

Hence, V is a minimizer in the Gagliardo–Nirenberg inequality. Moreover,

$$\|V\|_{L^2}^2 = 1 = \|v^n\|_{L^2}, \quad \|V\|_{\dot{H}_+^{1/2}}^2 = \pi = \lim_{n\to\infty} \|v^n\|_{\dot{H}_+^{1/2}}^2.$$

By (5-2) and (5-3), we have $r_n \to 0$ in $H_+^{1/2}$ as $n \to \infty$. Consequently, $v^n(\cdot + x_n) \to V$ in $H_+^{1/2}$, or equivalently,

$$\lim_{n\to\infty} \left\| a_n u^n(t_n, \lambda_n x) - V(x - x_n) \right\|_{H_+^{1/2}} = 0.$$

We then have

$$\lim_{n\to\infty} \left\| u^n(t_n, x) - \frac{1}{a_\infty} V\left(\frac{x - x_n\lambda_\infty}{\lambda_\infty}\right) \right\|_{H_+^{1/2}} = 0.$$

Notice that, since V is a minimizer in the Gagliardo–Nirenberg inequality, we have

$$\tilde{\phi}(x) := \frac{1}{a_\infty} V\left(\frac{x}{\lambda_\infty}\right) = \frac{\alpha}{x - p} \in C(a, r).$$

Then, since $x_n\lambda_\infty \in \mathbb{R}$, we have $\phi(x) = \tilde{\phi}(x - x_n\lambda_\infty) = \dfrac{\alpha}{x - \tilde{p}} \in C(a, r)$. Thus,

$$\inf_{\phi\in C(a,r)} \|u^n(t_n, x) - \phi(x)\|_{H_+^{1/2}} \to 0, \text{ as } n \to \infty. \tag{5-4}$$

The conclusion follows by approximating the supremum in the statement by the sequence in (5-4) with an appropriate $\{t_n\}_{n\in\mathbb{N}}$. □

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SCATTERING THRESHOLD FOR THE FOCUSING NONLINEAR KLEIN–GORDON EQUATION

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We show scattering versus blow-up dichotomy below the ground state energy for the focusing nonlinear Klein–Gordon equation, in the spirit of Kenig and Merle for the H^1 critical wave and Schrödinger equations. Our result includes the H^1 critical case, where the threshold is given by the ground state for the massless equation, and the 2D square-exponential case, where the mass for the ground state may be modified, depending on the constant in the sharp Trudinger–Moser inequality. The main difficulty is the lack of scaling invariance in both the linear and the nonlinear terms.

A table of notation can be found on page 458.

1. Introduction

The problem and overview. We study global and asymptotic behavior of solutions in the energy space for the nonlinear Klein–Gordon equation (NLKG):

$$\ddot{u} - \Delta u + u = f'(u), \quad u : \mathbb{R}^{1+d} \to \mathbb{R} \quad (d \in \mathbb{N}), \tag{1-1}$$

where $f : \mathbb{R} \to \mathbb{R}$ is a given function. Typical examples that we can treat are the power nonlinearities in any dimension:

$$f(u) = \lambda |u|^{p+2} \quad (2_\star < p+2 \le 2^\star, \quad \lambda \ge 0), \tag{1-2}$$

where $2_\star$ and $2^\star$ respectively denote the L^2 and H^1 critical powers

$$2_\star = 2 + \frac{4}{d}, \quad 2^\star = \begin{cases} 2 + \dfrac{4}{d-2} & \text{if } d \ge 3, \\ \infty & \text{if } d \le 2, \end{cases} \tag{1-3}$$

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and the square-exponential nonlinearity in two spatial dimensions:

$$f(u) = \lambda|u|^p e^{\kappa|u|^2}, \quad (d = 2,\ p > 4,\ \lambda \geq 0,\ \kappa > 0), \tag{1-4}$$

which is related to the critical case for the Trudinger–Moser inequality. The equation conserves (at least formally) the energy

$$E(u;t) = E(u(t), \dot{u}(t)) := \int_{\mathbb{R}^d} \frac{|\dot{u}|^2 + |\nabla u|^2 + |u|^2}{2} - f(u)\,dx. \tag{1-5}$$

The main goal in this paper is to give necessary and sufficient conditions for the solution u to scatter, which means that u is asymptotic to some free solutions as $t \to \pm\infty$, under the condition that u has less energy than the least energy static solution, namely the ground state. In the defocusing case, where f has the opposite sign, one has the scattering result for all finite energy solutions, see [Brenner 1984; Ginibre and Velo 1985a; Nakanishi 1999a; 1999b; 2001; Ibrahim et al. 2009]. In the focusing case, it turns out that the solutions below the ground energy split into the scattering solutions and the blow-up solutions (in both time directions in both cases). Such results have been recently established for many other equations including the nonlinear wave equation (NLW), the nonlinear Schrödinger equation (NLS), the Yang–Mills system and the wave maps, since Kenig-Merle's [Kenig and Merle 2006] on NLS with the H^1 critical power (i.e. $p + 2 = 2^\star$ in (1-2)); see [Akahori and Nawa 2010; Côte et al. 2008; Duyckaerts et al. 2008; Kenig and Merle 2008; Killip et al. 2008; 2009; Krieger and Schlag 2009; Sterbenz and Tataru 2010; Tao 2008a; 2008b; 2008c; 2009a; 2009b].

To be more precise, let us recall the result by Kenig and Merle for the critical nonlinear wave equation

$$\ddot{u} - \Delta u = f'(u), \quad f(u) = |u|^{2^\star}. \tag{1-6}$$

Let $E^{(0)}(u)$ be the conserved energy, and Q be a static solution with the least energy:

$$E^{(0)}(u) := \int_{\mathbb{R}^d} \frac{|\dot{u}|^2 + |\nabla u|^2}{2} + f(u)\,dx, \quad Q(x) := \left[1 + \frac{|x|^2}{d(d-2)}\right]^{-(d-2)/2}. \tag{1-7}$$

Kenig and Merle [2008] proved that every solution with $E^{(0)}(u) < E^{(0)}(Q)$ scatters in the energy space as $t \to \pm\infty$, provided that $\|\nabla u(0)\|_{L^2} < \|\nabla Q\|_{L^2}$, and otherwise it blows up in finite time both for $t > 0$ and for $t < 0$. The idea of their proof is to bring the concentration compactness argument into the scattering problem by using space-time norms and the concept of a "critical element", that is, the minimal non-scattering solution.

The equations in those papers following Kenig and Merle have a common important property—the scaling invariance. It is further shared with the solution space (either the energy space or L^2, i.e. the critical case), except for the NLS with a subcritical power [Duyckaerts et al. 2008; Akahori and Nawa 2010]. The scaling invariance brings significant difficulties for the analysis, but also a lot of algebraic or geometric structures and simplifications. Hence it is a natural question what happens if the invariance is broken in the linear and the nonlinear parts of the equation. This is the main technical challenge in this paper.

The dichotomy into the global existence and the blow-up has been known long before the scattering result of Kenig and Merle, under the name of "potential well", defined by derivatives of the static energy functional. More precisely, Payne and Sattinger [1975] proved on bounded domains the dichotomy into blow-up and global existence for solutions below the ground energy, by the sign of the functional

$$K_{1,0}(u) := \int |\nabla u|^2 + |u|^2 - uf'(u)\,dx. \tag{1-8}$$

It is easy to observe that their argument applies to the whole space $\mathbb{R}^d$ as soon as one has the local wellposedness in the energy space. Hence our primary task is to prove the scattering result in the region of global existence. Then our first problem due to the inhomogeneity is that the above functional $K_{1,0}$ is not suited for the scattering proof, though it is useful for the blow-up and global existence. More specifically, we want to use the functional

$$K_{d,-2}(u) := \int 2|\nabla u|^2 + d[uf'(u) - 2f(u)]\,dx, \tag{1-9}$$

which is related to the virial identity. There is actually a one-parameter family of functionals, corresponding to various scalings, each of which defines a splitting of the solutions below the ground energy by its sign. For example, Shatah [1985] used another functional

$$K_{0,1}(u) := \int \frac{d-2}{2}|\nabla u|^2 + \frac{d}{2}|u|^2 - df(u)\,dx, \tag{1-10}$$

to prove the instability of the standing waves. Note that in his proof the instability is not given by blow-up in the region $K_{0,1}(u) < 0$. More recently, Ohta and Todorova [2007] proved blow-up in the region $K_{d,-2}(u) < 0$, but they need radial symmetry for the powers p close to $2^\star$.

The special feature of the critical wave Equation (1-6) is that those functionals are the same modulo constant multiples, which is exactly due to the scaling invariance. For the NLS with a subcritical power [Duyckaerts et al. 2008; Akahori and Nawa 2010], the functionals are different from each other, but the situation is much better than NLKG, because they contain only two terms (without the L^2 norm), the L^2 is another conserved quantity, and the virial identity is used both for the blow-up and for the scattering, while $K_{1,0}$ is not so useful for NLS.

It turns out, however, that those algebraically different functionals for NLKG define the same splitting below the threshold energy. This observation does not seem to be well recognized, but it is indeed crucial for the proof of the dichotomy, since we need different functionals for the blow-up and for the scattering.

One interesting feature resulting from the breakdown of the scaling is that, for some nonlinearity, the energy threshold is not given by the ground state of the original NLKG, but by that of a modified equation. More precisely, for the H^1 critical power ($p + 2 = 2^\star$) in three dimensions or higher, the threshold is given by that of the critical wave equation, or massless Klein–Gordon equation. This can be expected because the concentration by the critical scaling makes the L^2 norm vanish while preserving other components, namely the massless energy. However the transition from the Klein–Gordon to the wave requires some effort in the scattering proof.

We find another instance of mass modification, which is more surprising. That is in two dimensions and for nonlinearities which grow slightly slower than the square exponential $e^{|u|^2}$, where the mass for the threshold ground energy can change to any number between 0 and 1, depending on the constant in the sharp (L^2) Trudinger–Moser inequality. Thus we prove the existence of extremizers as well as the ground states with mass less than or equal to the sharp constant, which also seems new for general nonlinearity on the whole plane. For the existence of the ground state on bounded domains, we refer to [Figueiredo et al. 1995; Adimurthi 1990; Adimurthi and Struwe 2000]. One should be warned, however, that the situation on the whole plane is different from that on disks, unlike the higher dimensional Sobolev critical case, since here the concentration compactness has to be accompanied with a leak of L^2 norm to the spatial infinity. This will be discussed in [Ibrahim et al. 2011].

It is worth noting that the scattering result in the focusing exponential case is actually easier to obtain than in the defocusing case, concerning the global Strichartz estimate. This is because the (mass-modified) ground energy threshold implies that our solutions are in the subcritical regime for the Trudinger–Moser inequality. Hence concentration of energy is a priori precluded, and so we do not need the concentration radius or the localized Strichartz estimate used in [Ibrahim et al. 2009] on the Trudinger–Moser threshold in the defocusing case. This is another striking difference from the power case, where the analysis for the focusing case essentially contains that for the defocusing case.

Main result. To state the main results of this paper, we need to introduce some notation and assumptions for the variational setting and the nonlinear setting of the problem.

Variational setting. To specify our class of solutions, we need the static energy

$$J(\varphi) := \frac{1}{2}\int_{\mathbb{R}^d} [|\nabla\varphi|^2 + |\varphi|^2]\,dx - F(\varphi), \quad F(\varphi) := \int_{\mathbb{R}^d} f(\varphi)\,dx, \tag{1-11}$$

and its derivatives with respect to different scalings. In the critical and exponential cases, we also need the energy with a modified mass $c \geq 0$,

$$J^{(c)}(\varphi) = \frac{1}{2}\int_{\mathbb{R}^d} [|\nabla\varphi|^2 + c|\varphi|^2]\,dx - F(\varphi). \tag{1-12}$$

For any $\alpha, \beta, \lambda \in \mathbb{R}$ and $\varphi : \mathbb{R}^d \to \mathbb{R}$, we define the two-parameter rescaling family

$$\varphi^{\lambda}_{\alpha,\beta}(x) = e^{\alpha\lambda}\varphi(e^{-\beta\lambda}x), \tag{1-13}$$

and the differential operator $\mathscr{L}_{\alpha,\beta}$ acting on any functional $S : H^1(\mathbb{R}^d) \to \mathbb{R}$ by

$$\mathscr{L}_{\alpha,\beta} S(\varphi) = \frac{d}{d\lambda}\bigg|_{\lambda=0} S(\varphi^{\lambda}_{\alpha,\beta}). \tag{1-14}$$

The scaling derivative of the static energy is denoted by

$$\begin{aligned} K_{\alpha,\beta}(\varphi) &:= \mathscr{L}_{\alpha,\beta} J(\varphi) \\ &= \int_{\mathbb{R}^d} \left[\frac{2\alpha + (d-2)\beta}{2}|\nabla\varphi|^2 + \frac{2\alpha + d\beta}{2}|\varphi|^2 - \alpha\varphi f'(\varphi) - d\beta f(\varphi)\right] dx, \\ K^{(c)}_{\alpha,\beta}(\varphi) &:= \mathscr{L}_{\alpha,\beta} J^{(c)}(\varphi). \end{aligned} \tag{1-15}$$

For each $(\alpha, \beta) \in \mathbb{R}^2$ in the range

$$\alpha \geq 0, \quad 2\alpha + d\beta \geq 0, \quad 2\alpha + (d-2)\beta \geq 0, \quad (\alpha, \beta) \neq (0, 0), \tag{1-16}$$

we consider the constrained minimization problem

$$m_{\alpha,\beta} = \inf\{J(\varphi) \mid \varphi \in H^1(\mathbb{R}^d),\ \varphi \neq 0,\ K_{\alpha,\beta}(\varphi) = 0\}. \tag{1-17}$$

We will prove that it is attained, (after a modification of the mass in some cases), provided that (α, β) is in the above range (1-16). The condition on (α, β) is also necessary in general (see Proposition A.1).

Our solutions start from the following subsets of the energy space:

$$\begin{aligned} \mathcal{K}^+_{\alpha,\beta} &= \{(u_0, u_1) \in H^1(\mathbb{R}^d) \times L^2(\mathbb{R}^d) \mid E(u_0, u_1) < m_{\alpha,\beta},\ K_{\alpha,\beta}(u_0) \geq 0\}, \\ \mathcal{K}^-_{\alpha,\beta} &= \{(u_0, u_1) \in H^1(\mathbb{R}^d) \times L^2(\mathbb{R}^d) \mid E(u_0, u_1) < m_{\alpha,\beta},\ K_{\alpha,\beta}(u_0) < 0\}. \end{aligned} \tag{1-18}$$

Nonlinear setting. For the nonlinearity f, we consider the following three cases: the H^1 subcritical $(d \geq 1)$, the 2D exponential case, and the H^1 critical $(d \geq 3)$ cases. First we assume that $f : \mathbb{R} \to \mathbb{R}$ is C^2 and

$$f(0) = f'(0) = f''(0) = 0. \tag{1-19}$$

Secondly for the variational arguments, we need some monotonicity and convexity conditions. Let D denote the linear operator defined by

$$Df(u) := uf'(u). \tag{1-20}$$

We assume that f satisfies for some $\varepsilon > 0$,

$$(D - 2_\star - \varepsilon)f \geq 0, \quad (D - 2)(D - 2_\star - \varepsilon)f \geq 0, \tag{1-21}$$

which implies in particular that

$$D^2 f \geq (2_\star + \varepsilon)Df \geq (2_\star + \varepsilon)^2 f \geq 0. \tag{1-22}$$

Finally we need regularity and growth conditions, which can differ for small $|u|$ and large $|u|$. Fix a cut-off function $\chi \in C_0^\infty(\mathbb{R})$ satisfying $\chi(r) = 1$ for $|r| \leq 1$ and $\chi(r) = 0$ for $|r| \geq 2$, and set

$$\chi_R(x) := \chi(|x|/R), \tag{1-23}$$

for arbitrary vector x and $R > 0$. Decompose the nonlinearity by

$$f_S(u) := \chi_1(u) f(u), \quad f_L(u) = f(u) - f_S(u). \tag{1-24}$$

We assume that for some $p_1 > 2_\star - 2$

$$\begin{cases} |f_S''(u)| \lesssim |u|^{p_1} & (d \leq 4), \\ |f_S''(u_1) - f_S''(u_2)| \lesssim |u_1 - u_2|^{p_1} & (d \geq 5), \end{cases} \tag{1-25}$$

where we should choose $p_1 < 1$ for $d \geq 5$.

For the behavior of f for large $|u|$, we distinguish three cases:

(1) H^1 subcritical case: We assume that for some $p_2 < 2^\star - 2$

$$\begin{cases} |f_L''(u)| \lesssim |u|^{p_2} & (2 \leq d \leq 4) \\ |f_L''(u_1) - f_L''(u_2)| \lesssim (|u_1| + |u_2|)^{p_2 - 1}|u_1 - u_2| & (d \geq 5 \text{ and } p_2 \geq 1) \\ |f_L''(u_1) - f_L''(u_2)| \lesssim |u_1 - u_2|^{p_2} & (d \geq 5 \text{ and } p_2 < 1). \end{cases} \tag{1-26}$$

We allow $p_2 = 2^\star - 2$ in some of the later arguments. There is no growth restriction for $d = 1$. A typical example is

$$f(u) = \lambda_1 |u|^{q_1} + \cdots \lambda_k |u|^{q_k}, \tag{1-27}$$

where $\lambda_j > 0$ and $2_\star < q_j < 2^\star$ for all j, which satisfies (1-26) as well as (1-19), (1-21) and (1-25).

(2) H^1 critical case. We assume

$$d \geq 3, \quad f(u) = |u|^{2^\star}/2^\star. \tag{1-28}$$

In this case, we do not include lower powers in order to avoid their nontrivial effects in the variational characterization. The absence of lower powers will only be used in Section 2. In particular the Strichartz spaces we use in Section 4 can handle the sum of a critical power with a subcritical function.

(3) 2D exponential case: We assume that

$$\begin{aligned} &d = 2, \\ &\exists \kappa_0 \geq 0 \begin{Bmatrix} \forall \kappa > \kappa_0, \ \lim_{|u|\to\infty} f_L''(u) e^{-\kappa|u|^2} = 0 \\ \forall \kappa < \kappa_0, \ \lim_{|u|\to\infty} f_L(u) e^{-\kappa|u|^2} = \infty \end{Bmatrix} \text{ and if } \kappa_0 > 0 \text{ then } \lim_{|u|\to\infty} \frac{f_L(u)}{Df_L(u)} = 0. \end{aligned} \tag{1-29}$$

Then we define $C^\star_{\text{TM}}$ by

$$C^\star_{\text{TM}}(F) = \sup\bigl\{2F(\varphi)\|\varphi\|^{-2}_{L^2(\mathbb{R}^2)} \mid 0 \neq \varphi \in H^1(\mathbb{R}^2), \ \kappa_0 \|\nabla\varphi\|^2_{L^2(\mathbb{R}^2)} \leq 4\pi\bigr\}. \tag{1-30}$$

For example, all the conditions are satisfied by

$$f(u) = e^{\kappa_0|u|^2} - 1 - \kappa_0|u|^2 - \tfrac{1}{2}\kappa_0^2|u|^4 \tag{1-31}$$

and by

$$f(u) = |u|^p e^{\kappa_0|u|^2 + \gamma|u|}, \tag{1-32}$$

where $p > 4$, $\kappa_0 \geq 0$, and $\max(-\gamma, 0) \ll 1$ (depending on $\kappa_0(p-4)$). More specifically, it suffices to have for all $u \in [0, \infty)$ that

$$8\kappa_0 u^2 + 3\gamma u + 2(p-4) > 0, \tag{1-33}$$

since, putting $g := Df/f = 2\kappa_0 u^2 + \gamma u + p$, we have $2_\star = 4$ and

$$\begin{aligned} (D-2)(D-4)f &= [(g-4)^2 + Dg + 2(g-4)]f, \\ Dg + 2(g-4) &= 8\kappa_0 u^2 + 3\gamma u + 2(p-4) = 2[g(3u/2) - 4] - u^2/2. \end{aligned} \tag{1-34}$$

In addition, one can easily observe that $C^\star_{\text{TM}}(F) = \infty$ if $\gamma \geq 0$ and $C^\star_{\text{TM}}(F) < \infty$ if $\gamma < 0$, using Moser's sequence of functions for the former, and by the spherical symmetrization for the latter (compare [Moser 1971; Adachi and Tanaka 2000; Ruf 2005]).[1]

[1] Actually, the optimal (fastest) growth to have $C^\star_{\text{TM}}(F) < \infty$ is given by

$$f(u) \sim e^{\kappa_0|u|^2}/|u|^2 \quad (|u| \to \infty), \tag{1-35}$$

as shown in [Ibrahim et al. 2011]. The results in the present paper do not rely on this observation, though it seems to have its own interest.

In short, our assumption on f is that

$$(1\text{-}19),\ (1\text{-}21),\ (1\text{-}25),\ \text{and}\ [(1\text{-}26)\ \text{or}\ (1\text{-}28)\ \text{or}\ (1\text{-}29)]. \tag{1-36}$$

Then by Sobolev or Trudinger–Moser, we observe that F, $\mathcal{L}_{\alpha,\beta}F$ and $\mathcal{L}^2_{\alpha,\beta}F$ are continuous functionals on $H^1(\mathbb{R}^d)$.

Now we can state our main result. Denote the quadratic part of the energy (i.e., the linear energy) by

$$E^Q(u;t) = E^Q(u(t),\dot u(t)) := \int_{\mathbb{R}^d} \frac{|\dot u|^2 + |\nabla u|^2 + |u|^2}{2}\,dx. \tag{1-37}$$

Theorem 1.1. *Assume* (1-36) *for f. Then for all (α,β) in* (1-16), *both $m_{\alpha,\beta}$ and $\mathcal{K}^{\pm}_{\alpha,\beta}$ are independent of (α,β). Moreover* (1-1) *is locally wellposed in the energy space $H^1\times L^2$, and*

(1) *If $(u(0),\dot u(0)) \in \mathcal{K}^-_{\alpha,\beta}$, then u extends neither for $t\to\infty$ nor for $t\to-\infty$ as the unique strong solution in $H^1\times L^2$.*

(2) *If $(u(0),\dot u(0)) \in \mathcal{K}^+_{\alpha,\beta}$, then u scatters both in $t\to\pm\infty$ in the energy space. In other words, u is a global solution and there are $v_\pm$ satisfying*

$$\begin{aligned} &\ddot v_\pm - \Delta v_\pm + v_\pm = 0,\\ &E^Q(u-v_\pm, \dot u - \dot v_\pm) \to 0 \quad (t\to\pm\infty). \end{aligned} \tag{1-38}$$

The dichotomy of global existence versus blow-up in the subcritical case was essentially given in [Payne and Sattinger 1975], using $K_{1,0}$, on bounded domains. Hence our main contribution is the scattering part, and the parameter independence of $\mathcal{K}^{\pm}_{\alpha,\beta}$. The corresponding result in the defocusing case (hence only the scattering) has been shown in [Brenner 1984; Ginibre and Velo 1985b] for the subcritical f in three dimensions and higher, in [Nakanishi 1999b] in lower dimensions, in [Nakanishi 1999a] for the H^1 critical f, and in [Ibrahim et al. 2009] for the 2D exponential nonlinearity. The massless H^1 critical case (the other powers cannot be controlled by the massless energy) was solved by [Bahouri and Shatah 1998; Bahouri and Gérard 1999] for the defocusing f and by [Kenig and Merle 2008] for the focusing nonlinearity.

The parameter independence of $m_{\alpha,\beta}$ seems to be known in the study of stability of standing waves, but the authors could not find an available result as general as the above one. See [Ohta and Todorova 2007; Zhang 2002] for partial results. We quote a recent paper [Jeanjean and Le Coz 2009] for a pure power nonlinearity, but unfortunately their range of (α,β) was not correct (the condition $\alpha\ge 0$ was overlooked; its necessity is shown by Proposition A.1).

The parameter independence of $\mathcal{K}^{\pm}_{\alpha,\beta}$, on the other hand, does not seem to have got much attention from the stability analysis, but it is essential in our proof of the scattering, since the monotonicity is given for the blow-up and for the scattering in terms of different $K_{\alpha,\beta}$, respectively $K_{1,0}$ and $K_{d,-2}$.

Thanks to the parameter independence, we may write

$$m = m_{\alpha,\beta} \quad \text{and} \quad \mathcal{K}^{\pm} = \mathcal{K}^{\pm}_{\alpha,\beta}.$$

We will also show the following important properties of the energy threshold.

Proposition 1.2. *Let the assumptions be as in Theorem 1.1.*

(1) *In the subcritical case* (1-26), *the threshold energy m is attained by some $Q \in H^1(\mathbb{R}^d)$, independent of (α, β), solving the static equation*

$$-\Delta Q + Q = f'(Q), \tag{1-39}$$

with the least energy $J(Q) = m$ among the solutions in $H^1(\mathbb{R}^d)$. In other words, m is attained by the ground states.

(2) *In the critical case* (1-28), *there is no minimizer for* (1-17), *but we have*

$$m = J^{(0)}(Q), \tag{1-40}$$

for a static solution $Q \in \dot{H}^1(\mathbb{R}^d)$ of the massless equation

$$-\Delta Q = f'(Q), \tag{1-41}$$

with the least massless energy $J^{(0)}$. In other words, m equals the massless ground energy.

(3) *In the exponential case* (1-29), *let*

$$c := \min(1, C^{\star}_{\mathrm{TM}}(F)),$$

where $C^{\star}_{\mathrm{TM}}(F)$ is as in (1-30). *Then*

$$m = J^{(c)}(Q), \tag{1-42}$$

for a static solution $Q \in H^1(\mathbb{R}^2)$ of the mass-modified equation

$$-\Delta Q + cQ = f'(Q), \tag{1-43}$$

with the least energy $J^{(c)}(Q)$. Moreover we have

$$m \le 2\pi/\kappa_0, \tag{1-44}$$

where the equality holds if and only if $C^{\star}_{\mathrm{TM}}(F) \le 1$, and $m = m_{\alpha,\beta}$ is attained in (1-17) *if and only if $C^{\star}_{\mathrm{TM}}(F) \ge 1$.*

Again this is well known in the subcritical case. Hence the main novelty is in the mass change in the critical and exponential cases. Note that the ground state Q with a different mass $c \in [0, 1)$ yields standing wave solutions $e^{\pm it\omega} Q(x)$ with $1 - \omega^2 = c$. But it is not a true obstruction for the scattering, because its dynamical energy is above m, although m is the right threshold in the sense that for higher energy level $E > m$ the sets $\mathcal{K}^{\pm}$ are no longer separated from each other, that is, $\partial\mathcal{K}^+ \cap \partial\mathcal{K}^- \neq \varnothing$.

Some notation. We recall some standard notation. $\mathcal{F}$ denotes the Fourier transform on $\mathbb{R}^d$, and

$$\langle\nabla\rangle := \sqrt{1-\Delta} = \mathcal{F}^{-1}\sqrt{1+|\xi|^2}\,\mathcal{F}. \tag{1-45}$$

L^p, H^s, $B^s_{p,q}$ and $\dot B^s_{p,q}$ respectively denote the Lebesgue, Sobolev, inhomogeneous and homogeneous Besov spaces on $\mathbb{R}^d$. For later use we recall the most used functionals $K_{\alpha,\beta}$ and $H_{\alpha,\beta}$:

$$\begin{aligned} K_{1,0}(\varphi) &= \int_{\mathbb{R}^d} \big[|\nabla\varphi|^2 + |\varphi|^2 - \varphi f'(\varphi)\big]\,dx, \\ K_{0,1}(\varphi) &= \int_{\mathbb{R}^d} \Big[\frac{d-2}{2}|\nabla\varphi|^2 + \frac{d}{2}|\varphi|^2 - d f(\varphi)\Big]\,dx, \\ K_{d,-2}(\varphi) &= \int_{\mathbb{R}^d} \big[2|\nabla\varphi|^2 - d(D-2) f(\varphi)\big]\,dx, \end{aligned} \tag{1-46}$$

$$\begin{aligned} H_{1,0}(\varphi) &= \frac{1}{2}\int_{\mathbb{R}^d} [(D-2) f(\varphi)]\,dx, \\ H_{0,1}(\varphi) &= \int_{\mathbb{R}^d} \Big[\frac{1}{d}|\nabla\varphi|^2\Big]\,dx, \\ H_{d,-2}(\varphi) &= \int_{\mathbb{R}^d} \Big[\frac{1}{2}|\varphi|^2 + \frac{d}{4}(D-2_*) f(\varphi)\Big]\,dx. \end{aligned} \tag{1-47}$$

We give a table of notation on page 458.

2. Variational characterizations

In this section, we prove Proposition 1.2. In particular we prove the existence of ground states as constrained minimizers, the (α,β)-independence of the splittings, together with various estimates for solutions below the threshold by variational arguments, which will be used for the scattering and blowup.

Throughout this section, we assume that (α,β) is in the range (1-16). For ease of presentation, we often omit (α,β) from the subscript. We associate with it the following two numbers:

$$\bar\mu = \max(2\alpha + d\beta, 2\alpha + (d-2)\beta), \quad \underline{\mu} = \min(2\alpha + d\beta, 2\alpha + (d-2)\beta), \tag{2-1}$$

which come from the scaling exponents for $\dot H^1$ and L^2 in (1-13). Notice that in the range (1-16), we have $\bar\mu > 0$, $\underline{\mu} \ge 0$, and that $\alpha = \underline{\mu} = 0$ if and only if $(d,\alpha) = (2,0)$, which will often be an exceptional case in the following arguments.

We decompose $K_{\alpha,\beta} = \mathscr{L}_{\alpha,\beta} J$ into the quadratic and the nonlinear parts:

$$K_{\alpha,\beta} = K^Q_{\alpha,\beta} + K^N_{\alpha,\beta}, \quad K^Q_{\alpha,\beta}(\varphi) = \mathscr{L}_{\alpha,\beta}\|\varphi\|^2_{H^1}/2, \quad K^N_{\alpha,\beta}(\varphi) = -\mathscr{L}_{\alpha,\beta} F(\varphi). \tag{2-2}$$

Then $K^Q_{\alpha,\beta}(\varphi^\lambda_{\alpha,\beta})$ is non-negative and non-decreasing with respect to $\lambda \in \mathbb{R}$, and

$$\lim_{\lambda\to-\infty} K^Q_{\alpha,\beta}(\varphi^\lambda_{\alpha,\beta}) = 0, \tag{2-3}$$

from its explicit form.

Energy landscape in various scales. First we investigate how J and its derivatives behave with respect to the scaling $\varphi^\lambda_{\alpha,\beta}$, in order to get $m_{\alpha,\beta}$ as a minimax value. The results of this subsection are essentially known, at least under more restrictions on the nonlinearity and (α,β).

We start from the origin of the energy space.

Lemma 2.1 (Positivity of K near 0). *Assume that f satisfies* (1-36), *and that* (α,β) *satisfies* (1-16) *and* $(d,\alpha)\neq(2,0)$. *Then for any bounded sequence $\varphi_n\in H^1(\mathbb{R}^d)\setminus\{0\}$ such that $K^Q_{\alpha,\beta}(\varphi_n)\to 0$, we have, for large n,*

$$K_{\alpha,\beta}(\varphi_n)>0. \tag{2-4}$$

Note that if $(d,\alpha)=(2,0)$ the conclusion is false, since in that case $K^Q(\varphi^\lambda)=e^{d\beta\lambda}K^Q(\varphi)\to 0$ as $\lambda\to-\infty$, but $K(\varphi^\lambda)=e^{d\beta\lambda}K(\varphi)$ can be negative.

Proof. First we consider the H^1 subcritical/critical cases. If $d\ge 2$ then

$$|Df(\varphi)|+|f(\varphi)|\lesssim|\varphi|^{p_1+2}+|\varphi|^{p_2+2}, \tag{2-5}$$

for some $2_\star<p_1+2<p_2+2\le 2^\star$; hence, by the Gagliardo–Nirenberg inequality

$$\|\varphi\|^q_{L^q_x}\lesssim\|\nabla\varphi\|^{d(q/2-1)}_{L^2_x}\|\varphi\|^{d-q(d-2)/2}_{L^2_x}\quad(2\le q\le 2^\star), \tag{2-6}$$

we obtain

$$|F(\varphi)|+|\mathscr{L}F(\varphi)|\lesssim\sum_{q=p_1+2,\,p_2+2}\|\nabla\varphi\|^{d(q/2-1)}_{L^2_x}\|\varphi\|^{d-q(d-2)/2}_{L^2_x}. \tag{2-7}$$

If $d=1$ then we can dispose of f_L by Sobolev $H^1(\mathbb{R})\subset L^\infty(\mathbb{R})$. Then we get

$$|F(\varphi)|+|\mathscr{L}F(\varphi)|\lesssim\|\nabla\varphi\|^{p_1/2+1}_{L^2_x}\|\varphi\|^{p_1/2+1}_{L^2_x}C(\|\varphi\|_{H^1}), \tag{2-8}$$

for some function C determined by f_L.

Hence if $2\alpha+(d-2)\beta>0$ then for any d we have

$$|K^N(\varphi)|=o(\|\nabla\varphi\|^2_{L^2_x})=o(K^Q(\varphi)). \tag{2-9}$$

Under the assumption, $2\alpha+(d-2)\beta=0$ is possible only for $d=1$; then, using (2-8),

$$|K^N(\varphi)|=o(\|\varphi\|^2_{L^2_x})=o(K^Q(\varphi)). \tag{2-10}$$

Finally we consider the 2D exponential case (1-29). Then we have

$$|Df(\varphi)|+|f(\varphi)|\lesssim|\varphi|^p(e^{\kappa|\varphi|^2}-1), \tag{2-11}$$

for some $p>2$ and any $\kappa>\kappa_0$. Since $\alpha>0$, we have $K^Q(\varphi_n)\gtrsim\|\nabla\varphi_n\|^2_{L^2}\to 0$, so it suffices to consider $\varphi\in H^1$ satisfying, for some $q>1$ such that $(4-p)q<2$,

$$q\kappa\|\nabla\varphi\|^2_{L^2}\le 2\pi. \tag{2-12}$$

Let $q'=q/(q-1)$ be the Hölder conjugate. Then by Hölder, Gagliardo–Nirenberg (2-6) and the Trudinger–Moser inequality

$$\|\nabla\varphi\|_{L^2(\mathbb{R}^2)}<\sqrt{4\pi}\implies\int_{\mathbb{R}^2}(e^{|\varphi|^2}-1)\,dx\lesssim\frac{\|\varphi\|^2_{L^2(\mathbb{R}^2)}}{4\pi-\|\nabla\varphi\|^2_{L^2(\mathbb{R}^2)}}, \tag{2-13}$$

we obtain

$$
\begin{aligned}
|\mathcal{L}F(\varphi)|+|F(\varphi)| \lesssim \|\varphi\|_{L^{pq'}}^{p}\|e^{q\kappa|\varphi|^2}-1\|_{L^1}^{1/q} \lesssim \|\varphi\|_{L^2}^{2/q'}\|\nabla\varphi\|_{L^2}^{p-2/q'}\left[\frac{\|\varphi\|_{L^2}^2}{4\pi-q\kappa\|\nabla\varphi\|_{L^2}^2}\right]^{1/q} \\
\lesssim \|\varphi\|_{L^2}^2\|\nabla\varphi\|_{L^2}^{p-2/q'}.
\end{aligned} \tag{2-14}
$$

Since $p-2/q'>2$ by the choice of q, we get

$$
|K^N(\varphi)| = o(\|\nabla\varphi\|_{L^2}^2) = o(K^Q(\varphi)). \tag{2-15}
$$

Thus in all cases $K(\varphi)\sim K^Q(\varphi)>0$ when $0<K^Q(\varphi)\ll 1$. □

The following inequalities describe the graph of J, and will play the central role in the succeeding arguments.

Lemma 2.2 (Mountain-pass structure). *Assume that f satisfies* (1-36) *and (α,β) satisfies* (1-16). *Then for any $\varphi\in H^1(\mathbb{R}^d)$ we have*

$$
\begin{aligned}
(\mathcal{L}_{\alpha,\beta}-\bar{\mu})\|\varphi\|_{H^1}^2 &\le -2|\beta|\min(\|\varphi\|_{L^2}^2,\|\nabla\varphi\|_{L^2}^2), \\
(\mathcal{L}_{\alpha,\beta}-\bar{\mu})F(\varphi) &\ge \alpha\varepsilon F(\varphi),
\end{aligned} \tag{2-16}
$$

where $\varepsilon>0$ is given in (1-21). *Hence*

$$
(\bar{\mu}-\mathcal{L}_{\alpha,\beta})J(\varphi) \ge \alpha\varepsilon F(\varphi)+|\beta|\min(\|\varphi\|_{L^2}^2,\|\nabla\varphi\|_{L^2}^2). \tag{2-17}
$$

Moreover we have

$$
-(\mathcal{L}_{\alpha,\beta}-\bar{\mu})(\mathcal{L}_{\alpha,\beta}-\underline{\mu})J(\varphi) = (\mathcal{L}_{\alpha,\beta}-\bar{\mu})(\mathcal{L}_{\alpha,\beta}-\underline{\mu})F(\varphi) \ge \frac{2\alpha\varepsilon}{d+1}\mathcal{L}_{\alpha,\beta}F(\varphi) \ge \frac{2\alpha\varepsilon\bar{\mu}}{d+1}F(\varphi). \tag{2-18}
$$

Proof. First we observe that

$$
(\mathcal{L}-2\alpha-(d-2)\beta)\|\nabla\varphi\|_{L_x^2}^2 = 0, \quad (\mathcal{L}-2\alpha-d\beta)\|\varphi\|_{L_x^2}^2 = 0, \tag{2-19}
$$

and for any functional S of the form $S(\varphi)=\int_{\mathbb{R}^d} s(\varphi)\,dx$,

$$
\mathcal{L}_{\alpha,\beta}S(\varphi) = \int_{\mathbb{R}^d}[(\alpha D+\beta d)s](\varphi)\,dx, \tag{2-20}
$$

where $Df(\varphi)=\varphi f'(\varphi)$ as defined in (1-20). Using this, we obtain

$$
(\mathcal{L}-\bar{\mu})\|\varphi\|_{H^1}^2 = -2|\beta|\times\begin{cases}\|\nabla\varphi\|_{L^2}^2 & (\beta\ge 0),\\ \|\varphi\|_{L^2}^2 & (\beta\le 0),\end{cases} \tag{2-21}
$$

and also

$$
\mathcal{L}F(\varphi) = \int[\alpha(D-2)+2\alpha+d\beta]f(\varphi)\,dx = \int[(\alpha D-2\alpha+2\beta)+2\alpha+(d-2)\beta]f(\varphi)\,dx. \tag{2-22}
$$

Since

$$
\alpha D-2\alpha+2\beta = \alpha(D-2_\star)+\frac{2}{d}(2\alpha+d\beta), \tag{2-23}
$$

using (1-21), we obtain

$$
\mathcal{L}F \ge (\bar{\mu}+\alpha\varepsilon)F. \tag{2-24}
$$

Using these computations, we have

$$
\begin{aligned}
-(\mathscr{L}-\bar{\mu})(\mathscr{L}-\underline{\mu})J(\varphi) &= (\mathscr{L}-\bar{\mu})(\mathscr{L}-\underline{\mu})F(\varphi) \\
&= \alpha \int (\alpha D - 2\alpha + 2\beta)(D-2) f(\varphi)\, dx \\
&\geq \alpha\varepsilon \int \Big[\alpha(D-2) + \frac{2}{d}(2\alpha + d\beta)\Big] f(\varphi)\, dx \\
&\geq \frac{2}{d+1}\alpha\varepsilon\mathscr{L}F(\varphi) \geq \frac{2\alpha\varepsilon\bar{\mu}}{d+1}F(\varphi),
\end{aligned}
\tag{2-25}
$$

where we used (2-23) and (1-21) in the first inequality, $\min(1, 2/d) \geq 2/(d+1)$ in the second, and (2-24) in the last. ☐

Using the inequalities above, we can replace the minimized quantity in (1-17) with a positive definite one, while extending the minimizing region from "the mountain ridge" to "the mountain flank". Let

$$
H_{\alpha,\beta} := (1 - \mathscr{L}_{\alpha,\beta}/\bar{\mu})J. \tag{2-26}
$$

Then Lemma 2.2 implies that $H_{\alpha,\beta} > 0$ and

$$
\mathscr{L}_{\alpha,\beta}H_{\alpha,\beta} = -(\mathscr{L}-\underline{\mu})(\mathscr{L}-\bar{\mu})J/\bar{\mu} + \underline{\mu}(1-\mathscr{L}/\bar{\mu})J \geq \frac{2\alpha\varepsilon}{d+1}F + \underline{\mu}H_{\alpha,\beta} \geq 0. \tag{2-27}
$$

We can rewrite the minimization problem (1-17) by using H:

Lemma 2.3 (Minimization of H). *Assume that f satisfies* (1-36) *and* (α, β) *satisfies* (1-16). *Then $m_{\alpha,\beta}$ in* (1-17) *equals*

$$
m_{\alpha,\beta} = \inf\{H_{\alpha,\beta}(\varphi) \mid \varphi \in H^1(\mathbb{R}^d),\ \varphi \neq 0,\ K_{\alpha,\beta}(\varphi) \leq 0\}. \tag{2-28}
$$

Proof. Let m' denote the right side of (2-28). Then $m \geq m'$ is trivial because $J = H$ if $K = 0$, so it suffices to show $m \leq m'$. Take $\varphi \in H^1$ such that $K(\varphi) < 0$.

If $(d, \alpha) \neq (2, 0)$, then from Lemma 2.1 together with (2-3), we deduce that

$$
(d,\alpha) \neq (2,0),\ K(\varphi) < 0 \implies \exists\lambda < 0,\ K(\varphi^\lambda) = 0,\ H(\varphi^\lambda) \leq H(\varphi), \tag{2-29}
$$

where the latter inequality follows from (2-27) since $H(\varphi^\lambda)$ is nondecreasing in λ. Hence $m \leq m'$.

If $(d,\alpha) = (2,0)$, then we use another scaling νu with $\nu \in (0,1)$. We have $K^Q(\nu\varphi) = \nu^2 K^Q(\varphi)$ and $|K^N(\nu\varphi)| = o(\nu^4)$ by (2-7) or (2-14). Hence $K(\nu\varphi) > 0$ for small $\nu > 0$, and so we deduce

$$
(d,\alpha) = (2,0),\ K(\varphi) < 0 \implies \exists\nu \in (0,1),\ K(\nu\varphi) = 0,\ H(\nu\varphi) \leq H(\varphi), \tag{2-30}
$$

where the inequality follows from $H(\varphi) = \|\nabla\varphi\|_{L^2_x}^2/2$ in this case. Hence $m \leq m'$. ☐

The ground state as common minimizer. Now we can prove the parameter independence of $m_{\alpha,\beta}$ via its characterization by the ground states. First we consider the H^1 subcritical case.

Lemma 2.4 (Ground state in the subcritical case). *Assume that f satisfies* (1-36) *and* (1-26), *and that* (α, β) *satisfies* (1-16). *Then $m_{\alpha,\beta}$ in* (1-17) *is positive and independent of* (α,β). *Moreover $m_{\alpha,\beta} = J(Q)$ for some $Q \in H^1(\mathbb{R}^d)$ solving the static NLKG* (1-39) *with the minimal $J(Q)$ among the solutions in $H^1(\mathbb{R}^d)$.*

Proof. Let $\varphi_n \in H^1$ be a minimizing sequence for (2-28), namely $K(\varphi_n) \le 0$, $\varphi_n \ne 0$ and $H(\varphi_n) \searrow m$.

First we consider the case $(d,\alpha) \ne (2,0)$. Let φ_n^* be the Schwartz symmetrization of φ_n, i.e. the radial decreasing rearrangement. Since the symmetrization preserves the nonlinear parts and does not increase the $\dot H^1$ part, we have $\varphi_n^* \ne 0$, $K(\varphi_n^*) \le K(\varphi_n) \le 0$ and $H(\varphi_n) \ge H(\varphi_n^*) \to m$. Then using (2-29), we may replace it by symmetric $\psi_n \in H^1$ such that

$$\psi_n \ne 0, \quad K(\psi_n) = 0, \quad J(\psi_n) = H(\psi_n) \to m. \tag{2-31}$$

If $\alpha > 0$, then (2-17) implies

$$(\bar\mu + \alpha\varepsilon) J(\psi_n) \ge \alpha\varepsilon \|\psi_n\|_{H^1}^2/2; \tag{2-32}$$

hence ψ_n is bounded in H^1.

If $\alpha = 0$ (and $d > 2$), then $H(\psi_n) = \|\nabla\psi_n\|_{L_x^2}^2/d$ is bounded, and if $\|\psi_n\|_{L^2} \to \infty$, then by (2-7)

$$d\beta\|\psi_n\|_{L^2}^2 \le 2K^Q(\psi_n) = -2K^N(\psi_n) \le o(\|\psi_n\|_{L^2}^{d-2_\star(d-2)/2}), \tag{2-33}$$

but since $d - 2_\star(d-2)/2 < 2$, this is a contradiction. Hence ψ_n is bounded in H^1.

Since ψ_n is bounded in H^1, after replacing with some appropriate subsequence, it converges to some ψ weakly in H^1. By the radial symmetry, it also converges strongly in L^p for all $2 < p < 2^\star$. Then in the subcritical case (1-26), the nonlinear parts converge, and so $K(\psi) \le 0$ and $H(\psi) \le m$.

If $\psi = 0$, then $K(\psi_n) = 0$ implies that $K^Q(\psi_n) = -K^N(\psi_n) \to 0$, and by Lemma 2.1 we have $K(\psi_n) > 0$ for large n, a contradiction. Hence $\psi \ne 0$.

By (2-29), we may replace ψ by its rescaling, so that $K(\psi) = 0$, $J(\psi) = H(\psi) \le m$ and $\psi \ne 0$. Then ψ is a minimizer and $m = H(\psi) > 0$.

Since ψ is a minimizer for (1-17), there is a Lagrange multiplier $\eta \in \mathbb{R}$ such that

$$J'(\psi) = \eta K'(\psi). \tag{2-34}$$

Then denoting $\mathscr{L}\psi = \partial_\lambda \psi_{\alpha,\beta}^\lambda|_{\lambda=0}$, we get

$$0 = K(\psi) = \mathscr{L}J(\psi) = \langle J'(\psi) \mid \mathscr{L}\psi\rangle = \eta\langle K'(\psi) \mid \mathscr{L}\psi\rangle = \eta\mathscr{L}^2 J(\psi). \tag{2-35}$$

By (2-18) and $\mathscr{L}J(\psi) = 0$, we have

$$\mathscr{L}^2 J(\psi) \le -\bar\mu\underline{\mu} J(\psi) - \frac{2\alpha\varepsilon\bar\mu}{d+1} F(\psi) < 0, \tag{2-36}$$

since $\underline{\mu} > 0$ or $\alpha > 0$.

Therefore $\eta = 0$ and ψ is a solution to (1-39). The minimality of $J(\psi)$ among the solutions is clear from (1-17), since every solution Q in H^1 of (1-39) satisfies $K(Q) = \langle J'(Q) \mid \mathscr{L}Q\rangle = 0$. This implies that $m_{\alpha,\beta}$ is independent of (α,β).

In the exceptional case $(d,\alpha) = (2,0)$, the above argument needs considerable modifications, due to the scaling invariance

$$H(\varphi) = \|\nabla\varphi\|_{L^2}^2/2 = H(\varphi^\lambda), \quad K(\varphi^\lambda) = e^{d\beta\lambda}K(\varphi). \tag{2-37}$$

First, we should use (2-30) instead of (2-29) to get ψ_n satisfying (2-31). Next, the invariance breaks the H^1 boundedness of ψ_n. But we are free to replace each ψ_n by its rescaling so that $\|\psi_n\|_{L^2} = 1$, without losing its properties (2-31). Then

$$1 = \|\psi_n\|_{L^2}^2 = 2F(\psi_n) \to 2F(\psi),$$

which clearly implies that the limit ψ is nonzero. By (2-30), we may replace ψ by its constant multiple, so that $K(\psi) = 0$, $J(\psi) = H(\psi) \le m$ and $\psi \ne 0$. Then ψ is a minimizer and $m = H(\psi) > 0$.

Finally, the invariance gives us $\mathscr{L}^2 J(\psi) = 0$ and the Lagrange multiplier η may be nonzero. In this case (2-34) is written

$$-\Delta\psi = (\eta d\beta - 1)[\psi - f'(\psi)]. \tag{2-38}$$

Since $\langle -\Delta\psi \mid \psi\rangle_{L^2_x} > 0$ and

$$\langle \psi - f'(\psi) \mid \psi\rangle_{L^2_x} = K_{0,2/d}(\psi) - \int (D-2) f(\psi)\, dx < 0, \tag{2-39}$$

we have $(\eta d\beta - 1) < 0$. Hence there exists $\lambda > 0$ such that ψ^λ solves the static NLKG (1-39), and it is also a minimizer. □

H^1 critical case; massless threshold. In the H^1 critical case (1-28), we still have the (α, β) independence, but $m_{\alpha,\beta}$ is equal to the massless energy of the massless ground state. This is a consequence of the invariance of the massless energy with respect to the $\dot H^1$ scaling.

Lemma 2.5 (Ground state in H^1 critical case). *Assume that f satisfies* (1-28), *and that (α, β) satisfies* (1-16). *Then $m_{\alpha,\beta}$ in* (1-17) *is positive and independent of* (α, β). *Moreover $m_{\alpha,\beta} = J^{(0)}(Q)$ for some $Q \in \dot H^1(\mathbb{R}^d)$ solving the static massless NLKG* (1-41), *with the minimal $J^{(0)}(Q)$ among the solutions in $\dot H^1(\mathbb{R}^d)$.*

Proof. Let H^w and K^w be the massless versions of H and K, respectively. Then

$$m = m^w := \inf\{H^w(\varphi) \mid \varphi \in H^1,\ K^w(\varphi) < 0\}. \tag{2-40}$$

Indeed, comparing this expression with (2-28), we easily get $m \ge m^w$ from $H^w \le H$ and $K^w < K$ if $2\alpha + d\beta > 0$. If $2\alpha + d\beta = 0$, then we may replace $K \le 0$ in (2-28) by $K < 0$, because for any nonzero $\varphi \in H^1$ satisfying $K(\varphi) \le 0$, we have by (2-18)

$$\mathscr{L}K(\varphi) \le \bar\mu K(\varphi) - \frac{2\alpha\varepsilon\bar\mu}{d+1} F(\varphi) < 0, \tag{2-41}$$

which implies that $K(\varphi^\lambda) < 0$ for all $\lambda > 0$, and so the set $K < 0$ is dense in the minimization set of (2-28). Hence $m \ge m^w$ in this case too.

To prove $m \le m^w$, let

$$\varphi^\nu = \varphi^\nu_{d/2-1,-1} \tag{2-42}$$

denote the $\dot H^1$ invariant scaling. Then $K(\varphi^\nu) \to K^w(\varphi)$ and $H(\varphi^\nu) \to H^w(\varphi)$ as $\nu \to \infty$. Hence if $K^w(\varphi) < 0$ then $K(\varphi^\nu) < 0$ for large ν, and so $m \le m^w$.

Due to the $\dot H^1$ scale invariance, $K^w_{\alpha,\beta}$ for all (α,β) are constant multiples of the same functional, and H^w is independent of (α,β), so is the minimization for m^w. In fact we have

$$m^w = \inf\{\|\nabla\varphi\|_{L^2}^2/d \mid \varphi\in H^1,\ \|\nabla\varphi\|_{L^2}^2 < \|\varphi\|_{L^{2^\star}}^{2^\star}\}. \tag{2-43}$$

By homogeneity and the scaling $\varphi\mapsto\nu\varphi$, this is equal to

$$\inf_{0\neq\varphi\in H^1}\frac{1}{d}\|\nabla\varphi\|_{L^2}^2\left[\frac{\|\nabla\varphi\|_{L^2}^2}{\|\varphi\|_{L^{2^\star}}^{2^\star}}\right]^{\frac{d-2}{2}} = \inf_{0\neq\varphi\in H^1}\frac{1}{d}\left[\frac{\|\nabla\varphi\|_{L^2}}{\|\varphi\|_{L^{2^\star}}}\right]^d = \frac{(C_S^\star)^{-d}}{d}, \tag{2-44}$$

where $C_S^\star$ denotes the best constant for the Sobolev inequality

$$\|\varphi\|_{L^{2^\star}} \le C_S^\star\|\nabla\varphi\|_{L^2}, \tag{2-45}$$

which is well known to be attained by the explicit $Q\in\dot H^1$ given by

$$Q(x) = \left[1+\frac{|x|^2}{d(d-2)}\right]^{-\frac{d-2}{2}}, \tag{2-46}$$

which solves (1-41). □

Exponential case; mass-modified threshold. In the 2D exponential case (1-29), the conclusion is somewhat intermediate between the above two cases. If $C^\star_{\mathrm{TM}}(F)\ge 1$ then $m_{\alpha,\beta}$ is achieved by a ground state, but if $C^\star_{\mathrm{TM}}(F)<1$ then we can still see $m_{\alpha,\beta}$ as the energy of a ground state to an equation (1-43) where the mass is changed to $c=\min(1, C^\star_{\mathrm{TM}}(F))\in(0,1)$.

Lemma 2.6 (Ground state in the exponential case). *Assume that f satisfies* (1-36) *and* (1-29), *and that (α,β) satisfies* (1-16). *Then $m_{\alpha,\beta}$ in* (1-17) *is independent of (α,β) and $0<m_{\alpha,\beta}\le 2\pi/\kappa_0$, where the second inequality is strict if and only if $C^\star_{\mathrm{TM}}(F)>1$. Moreover $m_{\alpha,\beta}=J^{(c)}(Q)$ with $c=\min(1,C^\star_{\mathrm{TM}}(F))$ for some $Q\in H^1(\mathbb{R}^2)$ solving the modified static NLKG* (1-43) *with the minimal $J^{(c)}(Q)$ among the solutions in $H^1(\mathbb{R}^2)$.*

For the proof, we prepare some notations and lemmas. For any functional G on $H^1(\mathbb{R}^2)$ and any $A>0$, we introduce the Trudinger–Moser ratio

$$C^A_{\mathrm{TM}}(G) := \sup\bigl\{2G(\varphi)\|\varphi\|_{L^2}^{-2} \mid 0\neq\varphi\in H^1(\mathbb{R}^2),\ \|\nabla\varphi\|_{L^2}\le A\bigr\}, \tag{2-47}$$

the Trudinger–Moser threshold on the $\dot H^1$ norm:

$$\mathfrak{M}(G) := \sup\{A>0 \mid C^A_{\mathrm{TM}}(G)<\infty\}, \tag{2-48}$$

and the ratio on the threshold:

$$C^\star_{\mathrm{TM}}(G) := C^{\mathfrak{M}(G)}_{\mathrm{TM}}(G). \tag{2-49}$$

The growth condition (1-29) together with (1-21) implies

$$\mathfrak{M}(\mathscr{L}_{\alpha,\beta}F) = \mathfrak{M}(F) = \sqrt{4\pi/\kappa_0} \tag{2-50}$$

for any (α,β) satisfying (1-16), by the Trudinger–Moser inequality (2-13). Hence the definition of $C^\star_{\mathrm{TM}}$ just given is consistent with (1-30).

For any functional G of the form $G(\varphi) = \int g(\varphi)\,dx$, and for any sequence $(\varphi_n)_{n\in\mathbb{N}} \in H^1(\mathbb{R}^2)^{\mathbb{N}}$, we define its concentration (at $x = 0$) $\operatorname{conc} G((\varphi_n)_{n\in\mathbb{N}})$ by

$$\operatorname{conc} G((\varphi_n)_{n\in\mathbb{N}}) := \varlimsup_{\varepsilon\to+0} \varlimsup_{n\to\infty} \int_{|x|<\varepsilon} g(\varphi_n)\,dx. \tag{2-51}$$

We will use the following compactness by dominated convergence.

Lemma 2.7. *Let $g, h : \mathbb{R} \to \mathbb{R}$ be continuous functions satisfying*

$$\lim_{u\to\pm\infty} \frac{|g(u)|}{h(u)} = 0, \quad \lim_{u\to 0} \frac{|g(u)|}{|u|^2} = 0. \tag{2-52}$$

Let φ_n be a sequence of radial functions, weakly convergent to φ in $H^1(\mathbb{R}^2)$ such that $\{h(\varphi_n)\}_n$ is bounded in $L^1(\mathbb{R}^2)$. Then $g(\varphi_n) \to g(\varphi)$ strongly in $L^1(\mathbb{R}^2)$.

Proof. By assumption (2-52), for any $\varepsilon > 0$ there exist $\delta > 0$ such that

$$|u| > 1/(2\delta) \text{ or } |u| < 2\delta \implies |g(u)| < \varepsilon(h(u) + |u|^2). \tag{2-53}$$

Then we have

$$\int_{|\varphi_n|>1/(2\delta) \text{ or } |\varphi_n|<2\delta} |g(\varphi_n)|dx \lesssim \varepsilon \int h(\varphi_n) + |\varphi_n|^2 dx \lesssim \varepsilon. \tag{2-54}$$

The radial Sobolev inequality $\|r^{1/2}\varphi_n\|_{L^\infty} \lesssim \|\varphi_n\|_{L^2}^{1/2} \|\nabla\varphi_n\|_{L^2}^{1/2}$ implies that $\varphi_n(x)$ are uniformly small for large x. Then the weak convergence together with

$$\varphi_n(R_1) - \varphi_n(R_2) = \int_{R_1}^{R_2} \partial_r \varphi_n(r)\,dr \tag{2-55}$$

implies that $\varphi_n(x) \to \varphi(x)$ for $x \neq 0$. Then Fatou's lemma implies

$$\int_{|\varphi|>1/(2\delta) \text{ or } |\varphi|<2\delta} |g(\varphi)|dx \lesssim \varepsilon, \tag{2-56}$$

and the dominated convergence theorem implies

$$\|g^{(\delta)}(\varphi_n) - g^{(\delta)}(\varphi)\|_{L^1} \to 0 \quad (n \to \infty), \tag{2-57}$$

where $g^{(\delta)}$ is defined by $g^{(\delta)}(u) = (1-\chi_\delta(u))\chi_{1/\delta}(u)g(u)$ using the cut-off defined in (1-23). Combining (2-54), (2-56) and (2-57), we deduce the desired convergence. □

Proof of Lemma 2.6. We start with the exceptional case $(d, \alpha) = (2, 0)$. First, let $A > 0$ and assume $C^A_{\mathrm{TM}}(F) > 1$. Then there exists $0 \neq \varphi \in H^1$ such that $\|\nabla\varphi\|_{L^2} \le A$ and $F(\varphi) > \|\varphi\|_{L^2}^2/2$. For small $\varepsilon > 0$ we have $K_{0,1}((1-\varepsilon)\varphi) < 0$, and hence $m_{0,1} \le \|\nabla(1-\varepsilon)\varphi_n\|_{L^2}^2/2 < A^2/2$. Hence $m_{0,1} \le \mathfrak{M}(F)^2/2$.

Consider the case $C^\star_{\mathrm{TM}}(F) > 1$. Then by choosing $A = \mathfrak{M}(F)$ in the above argument, we get $m_{0,1} < \mathfrak{M}(F)^2/2$. Now we take a minimizing sequence for $m_{0,1}$. By the Schwartz symmetrization and rescalings as in the proof of Lemma 2.4 for $(d, \alpha) = (2, 0)$, we get a sequence of radial functions $\psi_n \in H^1$ such that

$$\|\psi_n\|_{L^2} = 1, \quad H_{0,1}(\psi_n) \to m_{0,1}, \quad K_{0,1}(\psi_n) = 1 - 2F(\psi_n) = 0, \tag{2-58}$$

and $\psi_n \to \psi$ in H^1. Because of $m_{0,1} < \mathfrak{M}(F)^2/2$, we can choose some $\kappa \in (\kappa_0, 2\pi/m_{0,1})$, so that $e^{\kappa|\psi_n|^2} - 1$ is bounded in L^1 by the Trudinger–Moser inequality (2-13). Then we can use Lemma 2.7 with $\varphi_n := \psi_n$, $g := f$ and $h(u) := e^{\kappa|u|^2} - 1$, which implies $F(\psi_n) \to F(\psi)$. Hence ψ attains $m_{0,1}$. After appropriate rescalings, we obtain a ground state Q, as in the proof of Lemma 2.4.

Next consider the case $C^{\star}_{\mathrm{TM}}(F) \le 1$. Then for any $\psi \in H^1$ satisfying $\|\nabla\psi\|_{L^2} \le \mathfrak{M}(F)$ we have $K_{0,1}(\psi) \ge 0$. Hence

$$m_{0,1} = \inf\{\|\nabla\varphi\|_{L^2}^2/2 \mid K_{0,1}(\varphi) < 0\} \ge \mathfrak{M}(F)^2/2, \tag{2-59}$$

and so $m_{0,1} = \mathfrak{M}(F)^2/2$. Now we show that there exists $\varphi \in H^1$ satisfying

$$\|\nabla\varphi\|_{L^2} = \mathfrak{M}(F), \quad F(\varphi) = C^{\star}_{\mathrm{TM}}(F)/2, \quad \|\varphi\|_{L^2} = 1. \tag{2-60}$$

After rescaling this φ, we obtain a ground state Q. However, due to the criticality, we have to approximate the problem by a subcritical one, namely we first prove the existence of $\varphi_n \in H^1$ satisfying

$$\|\nabla\varphi_n\|_{L^2} \le \mathfrak{M}(F) - \frac{1}{n}, \quad F(\varphi_n) = c_n/2, \quad \|\varphi_n\|_{L^2} = 1 \tag{2-61}$$

where $c_n := C_{\mathrm{TM}}^{\mathfrak{M}(F)-\frac{1}{n}}(F)$; then $0 < c_n \nearrow C^{\star}_{\mathrm{TM}}(F) \le 1$. Fix $n \gg 1$ and let $\varphi^k \in H^1(\mathbb{R}^2)$ be a maximizing sequence for c_n (see (2-47)):

$$\|\nabla\varphi^k\|_{L^2} \le \mathfrak{M}(F) - \frac{1}{n}, \quad F(\varphi^k) \nearrow c_n/2, \quad \|\varphi^k\|_{L^2} = 1, \tag{2-62}$$

where the L^2 norm is normalized by the rescaling $\varphi^{\lambda}_{0,1}$. The Schwartz symmetrization enables us to assume that φ^k are radial functions, and convergent to some φ_n weakly in H^1, by extracting a subsequence. Moreover, we have $F(\varphi^k) \to F(\varphi_n) = c_n/2$, by Lemma 2.7 with $g := f$ and $h = e^{\kappa|u|^2} - 1$ for some $\kappa \in (\kappa_0, 4\pi/(\mathfrak{M}(F) - 1/n)^2)$.

Thus φ_n is a maximizer, which implies that $\|\varphi_n\|_{L^2} = 1$ and

$$-\eta\Delta\varphi_n = f'(\varphi_n) - c_n\varphi_n, \tag{2-63}$$

for a Lagrange multiplier $\eta(n) \in \mathbb{R}$. Multiplying it with φ_n, we obtain

$$\eta\|\nabla\varphi_n\|_{L^2}^2 = \int Df(\varphi_n)\,dx - c_n\|\varphi_n\|_{L^2}^2 = \int (D-2)f(\varphi_n)\,dx > 0, \tag{2-64}$$

since $(D-2)f > 0$. Hence $\eta > 0$, and so $Q_n(x) := \varphi_n(\eta^{1/2}x) \in H^1$ satisfies

$$\|\nabla Q_n\|_{L^2} \le \mathfrak{M}(F) - \frac{1}{n}, \quad -\Delta Q_n + c_n Q_n = f'(Q_n). \tag{2-65}$$

Now consider the limit $n \to \infty$. The equation for Q_n implies that $0 = K^{(c_n)}_{0,1}(Q_n) = K^{(c_n)}_{1,-1}(Q_n)$, so

$$c_n\|Q_n\|_{L^2}^2 = 2F(Q_n), \quad \|\nabla Q_n\|_{L^2}^2 = 2\int (D-2)f(Q_n)\,dx \ge 4F(Q_n), \tag{2-66}$$

where the last inequality follows from $(D-4)f \ge 0$. Since $\|\nabla Q_n\|_{L^2}$ is bounded and c_n is positive non-decreasing, we deduce that $\|Q_n\|_{L^2}$ and $\int Df(Q_n)\,dx$ are bounded as $n \to \infty$. Hence we may extract a subsequence so that Q_n converges to some Q weakly in H^1, and then apply Lemma 2.7 with $\varphi_n := Q_n$, $g = f'$ and $h := Df$. Then $f'(Q_n) \to f'(Q)$ strongly in L^1, and so Q solves

$$-\Delta Q + cQ = f'(Q), \quad c := C^{\star}_{\mathrm{TM}}(F). \tag{2-67}$$

This implies that

$$K^{(c)}_{0,1}(Q) = \langle J^{(c)\prime}(Q) \mid \mathscr{L}_{0,1} Q\rangle = 0, \tag{2-68}$$

namely $2F(Q) = c\|Q\|^2_{L^2}$. Hence Q is a maximizer for $C^{\mathfrak{M}(F)}_{\mathrm{TM}}(F)$ with a non-zero Lagrange multiplier, which implies that $\|\nabla Q\|_{L^2} = \mathfrak{M}(F)$. Thus $J^{(c)}(Q) = \mathfrak{M}(F)^2/2$ is unique for any solution Q of (2-67).

Next we consider $m_{\alpha,\beta}$ with $\alpha > 0$. If $m_{0,1} < \mathfrak{M}(F)^2/2$, then there exists a ground state Q, which satisfies $K_{\alpha,\beta}(Q) = 0$ for all (α,β). Hence $m_{\alpha,\beta} \le J(Q) = m_{0,1}$.

Otherwise, $m_{0,1} = \mathfrak{M}(F)^2/2 = \mathfrak{M}(\mathscr{L}F)^2/2$. For any $A > \mathfrak{M}(\mathscr{L}F)$, there exists a sequence $\varphi_n \in H^1$ satisfying

$$\|\nabla\varphi_n\|_{L^2} \le A, \quad \|\varphi_n\|_{L^2} \to 0, \quad \mathscr{L}F(\varphi_n) \to \infty. \tag{2-69}$$

Since $K(\varphi) = \alpha\|\nabla\varphi\|^2_{L^2} + (\alpha+\beta)\|\varphi\|^2_{L^2} - \mathscr{L}F(\varphi)$ and $\alpha > 0$, we can replace each φ_n with $\varphi_n(x/\nu_n)$ with some $\nu_n \to +0$, so that we have after the rescaling

$$\|\nabla\varphi_n\|_{L^2} \le A, \quad K(\varphi_n) = 0, \quad \|\varphi_n\|_{L^2} \to 0. \tag{2-70}$$

Hence

$$m_{\alpha,\beta} \le \varliminf_{n\to\infty} J(\varphi_n) \le A^2/2,$$

and so $m_{\alpha,\beta} \le \mathfrak{M}(\mathscr{L}F)^2/2 = m_{0,1}$. Thus in both cases we have $m_{\alpha,\beta} \le m_{0,1} \le \mathfrak{M}(F)^2/2$.

Now suppose that $m_{\alpha,\beta} < m_{0,1} \le \mathfrak{M}(F)^2/2$. As in the proof of Lemma 2.4 for $(d,\alpha) \ne (2,0)$, we may find a sequence of radial $\varphi_n \in H^1$ such that

$$K(\varphi_n) = 0, \quad H(\varphi_n) \searrow m. \tag{2-71}$$

Therefore there exists φ such that $\varphi_n \to \varphi$ weakly in H^1, and pointwise for $x \ne 0$.

Let $\psi_n = \varphi_n - \varphi$. Then $\psi_n \to 0$ weakly in H^1, and so

$$\lim_{n\to\infty} K^Q(\varphi_n) = \lim_{n\to\infty} K^Q(\psi_n) + K^Q(\varphi) = \lim_{n\to\infty} \mathscr{L}F(\varphi_n) = \operatorname{conc}\mathscr{L}F((\varphi_n)_n) + \mathscr{L}F(\varphi), \tag{2-72}$$

where the second identity is because $K(\varphi_n) = 0$, and the last one follows from $\varphi_n(x) \to \varphi(x)$ for $x \ne 0$ and the radial Sobolev inequality $\|r^{1/2}\varphi_n\|_{L^\infty} \lesssim \|\varphi_n\|_{H^1}$. Since $H(\varphi) \le m$ by Fatou's lemma, we have $K(\varphi) \ge 0$, otherwise there would be some $\lambda < 0$ such that $K(\varphi^\lambda) = 0$ and $H(\varphi^\lambda) < H(\varphi) \le m$, a contradiction. Thus $K^Q(\varphi) \ge \mathscr{L}F(\varphi)$, and so from (2-72), we deduce

$$\lim_{n\to\infty} K^Q(\psi_n) \le \operatorname{conc}\mathscr{L}F((\varphi_n)_n). \tag{2-73}$$

Since $\mathscr{L}F(\varphi_n)$ is bounded by (2-72), Lemma 2.7 with $h_n := (\alpha D + \beta d)f$ implies that $\operatorname{conc} F((\varphi_n)_n) = 0$. Hence by (2-73) and $(\mathscr{L} - \bar\mu)F \ge 0$, we get

$$\lim_{n\to\infty} K^Q(\psi_n) \le \operatorname{conc}(\mathscr{L}-\bar\mu)F((\varphi_n)_n) \le \lim_{n\to\infty} (\mathscr{L}-\bar\mu)F(\varphi_n). \tag{2-74}$$

On the other hand we have

$$m = \lim_{n\to\infty} H(\varphi_n) = \lim_{n\to\infty} H^Q(\psi_n) + H^Q(\varphi) + \lim_{n\to\infty} (\mathscr{L}-\bar{\mu})F(\varphi_n)/\bar{\mu}, \tag{2-75}$$

where $H^Q(\psi) := (1-\mathscr{L}/\bar{\mu})\|\psi\|_{H^1}^2/2$ denotes the quadratic part of H. Combining the above two, and discarding $H^Q(\varphi) \ge 0$, we obtain

$$\lim_{n\to\infty} \|\psi_n\|_{H^1}^2/2 \le m < \mathfrak{M}(F)^2/2 = 2\pi/\kappa_0. \tag{2-76}$$

Hence applying Lemma 2.7 to φ_n with $h(u) := e^{\kappa|u|^2}-1$ for some $\kappa \in (\kappa_0, 2\pi/m)$, we get $\mathscr{L}F(\varphi_n) \to \mathscr{L}F(\varphi)$, and so φ is a minimizer for $m_{\alpha,\beta}$. Indeed, we have

$$e^{\kappa|\varphi_n|^2} - 1 \le e^{C_{\kappa,\kappa'}|\varphi|^2} - 1 + e^{\kappa'|\psi_n|^2} - 1 \tag{2-77}$$

for some $\kappa' \in (\kappa, 2\pi/m)$ and constant $C_{\kappa,\kappa'} > 0$. Hence $h(\varphi_n)$ is uniformly bounded in L^1. Recall that for a fixed $\varphi \in H^1$, $e^{C_{\kappa,\kappa'}|\varphi|^2} - 1 \in L^1$.

Then as in the proof of Lemma 2.4, we obtain a ground state Q with $J(Q) = m_{\alpha,\beta} < m_{0,1}$, which is a contradiction since $K_{0,1}(Q) = 0$. Hence $m_{\alpha,\beta} = m_{0,1}$ for all (α, β) in the range (1-16). □

Remark 2.8. In the above argument for $(\alpha, \beta) = (0, 1)$ in the case $C^{\star}_{\mathrm{TM}}(F) \le 1$, we used a priori bounds on the ground state to get the compactness. For general sequences, we can have concentrating loss of compactness on the kinetic threshold $\|\nabla\varphi\|_{L^2} = \mathfrak{M}(F)$ if and only if f satisfies

$$\overline{\lim_{|u|\to\infty}}\, e^{-\kappa_0|u|^2}|u|^2 f(u) \in (0, \infty). \tag{2-78}$$

Lemma 2.6 implies that the concentration requires more energy than the (mass-modified) ground state. Similar phenomena have been observed in slightly different settings (either on a bounded domain or on the $H^1(\mathbb{R}^2)$ threshold, where $e^{\kappa_0|u|^2}$ appears as the critical growth instead of $e^{\kappa_0|u|^2}/|u|^2$, see [Carleson and Chang 1986; Flucher 1992; Ruf 2005]). More details about this issue, including the above concentration compactness, will be addressed in a forthcoming paper.

Parameter independence of the splitting. The (α, β)-independence of $\mathscr{K}^{\pm}_{\alpha,\beta}$ follows from that of $m_{\alpha,\beta}$ and contractivity of $\mathscr{K}^{+}_{\alpha,\beta}$.

Lemma 2.9 (Parameter independence of $\mathscr{K}^{\pm}$). *Assume that f satisfies* (1-36), *and that* (α, β) *satisfies* (1-16). *Then $\mathscr{K}^{\pm}_{\alpha,\beta}$ in* (1-18) *are independent of* (α, β).

Proof. Since $m_{\alpha,\beta}$ is independent of (α, β), we only need to see that the sign of K is independent under the threshold m. Also, we may restrict to the first component. For any $\delta \ge 0$, we define $\mathscr{K}^{\pm\delta}_{\alpha,\beta} \subset H^1$ by

$$\begin{aligned} \mathscr{K}^{+\delta}_{\alpha,\beta} &= \{\varphi \in H^1 \mid J(\varphi) < m-\delta,\ K_{\alpha,\beta}(\varphi) \ge 0\}, \\ \mathscr{K}^{-\delta}_{\alpha,\beta} &= \{\varphi \in H^1 \mid J(\varphi) < m-\delta,\ K_{\alpha,\beta}(\varphi) < 0\}. \end{aligned} \tag{2-79}$$

Then $(u_0, u_1) \in \mathscr{K}^{\pm}_{\alpha,\beta}$ if and only if $u_0 \in \mathscr{K}^{\pm\delta}_{\alpha,\beta}$ with $\delta = \|u_1\|_{L^2}^2/2$. In addition, the disjoint union $\mathscr{K}^{+\delta}_{\alpha,\beta} \cup \mathscr{K}^{-\delta}_{\alpha,\beta}$ is already independent of α and β. Hence it suffices to show the independence of $\mathscr{K}^{+\delta}_{\alpha,\beta}$.

First we consider the interior exponents satisfying $2\alpha + d\beta > 0$ and $2\alpha + (d-2)\beta > 0$. Then $\mathscr{K}^{+\delta}_{\alpha,\beta}$ is contracted to $\{0\}$ by the rescaling $\varphi \mapsto \varphi^{\lambda}$ with $0 \ge \lambda \to -\infty$. This is due to the following facts:

(1) $K(\varphi^\lambda) > 0$ is preserved as long as $J(\varphi^\lambda) < m$, by the definition of m.

(2) $J(\varphi^\lambda)$ does not increase as λ decreases, as long as $\mathscr{L}J(\varphi^\lambda) = K(\varphi^\lambda) > 0$.

(3) $\varphi^\lambda \to 0$ in H^1 as $\lambda \to -\infty$, since $2\alpha + d\beta > 0$ and $2\alpha + (d-2)\beta > 0$.

In particular, J cannot be negative on $\mathscr{K}^+_{\alpha,\beta}$, and so $\mathscr{K}^{+\delta}_{\alpha,\beta} = \varnothing$ for $\delta \geq m$. For $0 \leq \delta < m$, both $\mathscr{K}^{\pm\delta}_{\alpha,\beta}$ are open in H^1. It follows for $\mathscr{K}^{-\delta}$ from the definition, and for $\mathscr{K}^{+\delta}$ from the facts that $J(\varphi) < m$ and $K(\varphi) = 0$ imply $\varphi = 0$, and that a neighborhood of 0 is contained in $\mathscr{K}^{+\delta}$, which follows from (2-7), (2-8) or (2-14). Then the above argument of the scaling contraction shows that $\mathscr{K}^{+\delta}_{\alpha,\beta}$ is connected. Hence each $\mathscr{K}^{+\delta}_{\alpha,\beta}$ cannot be separated by $\mathscr{K}^{+\delta}_{\alpha',\beta'}$ and $\mathscr{K}^{-\delta}_{\alpha',\beta'}$ with any other (α', β') in the interior range. Since $\mathscr{K}^{+\delta}_{\alpha,\beta} \cap \mathscr{K}^{+\delta}_{\alpha',\beta'}$ contains 0, we conclude that $\mathscr{K}^{+\delta}_{\alpha,\beta} = \mathscr{K}^{+\delta}_{\alpha',\beta'}$.

Finally for (α, β) on the boundary $2\alpha + d\beta = 0$ or $2\alpha + (d-2)\beta = 0$, take a sequence (α_n, β_n) in the interior converging to (α, β). Then $K_{\alpha_n,\beta_n} \to K_{\alpha,\beta}$, and so

$$\mathscr{K}^{\pm\delta}_{\alpha,\beta} \subset \bigcup_n \mathscr{K}^{\pm\delta}_{\alpha_n,\beta_n}. \tag{2-80}$$

Since the right side is independent of the parameter, so is the left. ☐

Variational estimates. We conclude this section with a few estimates on the energy-type functionals, which will be important in the proof of the blow-up and the scattering. We start with the easy observation that the free energy and the nonlinear energy are equivalent in the set $\mathscr{K}^+$.

Lemma 2.10 (Free energy equivalence in $\mathscr{K}^+$). *Assume that f satisfies* (1-36). *Then for any $(u_0, u_1) \in H^1(\mathbb{R}^d) \times L^2(\mathbb{R}^d)$ we have*

$$K_{1,0}(u_0) \geq 0 \implies \begin{cases} J(u_0) \leq \|u_0\|^2_{H^1_x}/2 \leq (1 + d/2)J(u_0), \\ E(u_0, u_1) \leq E^Q(u_0, u_1) \leq (1 + d/2)E(u_0, u_1). \end{cases} \tag{2-81}$$

Proof. Since $(D - 2 - c)f(u) \geq 0$ with $c := 4/d > 0$ by (1-21), we have for any $(u_0, u_1) \in H^1 \times L^2$,

$$\begin{aligned} K_{1,0}(u_0) &= \|u_0\|^2_{H^1_x} - (2+c)F(u_0) - \int (D-2-c) f(u_0)dx \\ &\leq (2+c)J(u_0) - c\|u_0\|^2_{H^1_x}/2 = (2+c)E(u_0, u_1) - cE^Q(u_0, u_1) - \|\dot{u}\|^2_{L^2_x}, \end{aligned} \tag{2-82}$$

and hence we obtain the desired estimate. ☐

In the 2D exponential case, we have a sharper bound on the derivatives, which implies that $\mathscr{K}^+$ is in the subcritical regime for the Trudinger–Moser inequality.

Lemma 2.11 (Subcritical bound in $\mathscr{K}^+$ in the 2D exponential case). *Assume that f satisfies* (1-36) *and* (1-29). *Then for any $(u_0, u_1) \in \mathscr{K}^+$ we have*

$$\|\nabla u_0\|^2_{L^2} + \|u_1\|^2_{L^2} < 2m \leq \mathfrak{M}(F)^2 = 4\pi/\kappa_0. \tag{2-83}$$

Proof. Since $K_{0,1}(u_0) \geq 0$, we have

$$\|\nabla u_0\|^2_{L^2} + \|u_1\|^2_{L^2} \leq \|\nabla u_0\|^2_{L^2} + \|u_1\|^2_{L^2} + K_{0,1}(u_0) = 2E(u_0, u_1) < 2m. \qquad ☐$$

The next estimate gives a lower bound on $|K|$ under the threshold m, which will be important both for the blow-up and for the scattering.

Lemma 2.12 (Uniform bounds on K). *Assume that f satisfies* (1-21), *and that (α,β) satisfies* (1-16) *and $(d,\alpha)\neq(2,0)$. Then there exists $\delta>0$ determined by (α,β), d and ε in* (1-21), *such that for any $\varphi\in H^1$ with $J(\varphi)<m$ we have*

$$K_{\alpha,\beta}(\varphi)\geq\min(\bar{\mu}(m-J(\varphi)),\delta K^Q_{\alpha,\beta}(\varphi))\quad or\quad K_{\alpha,\beta}(\varphi)\leq-\bar{\mu}(m-J(\varphi)).\tag{2-84}$$

Note that if $(d,\alpha)=(2,0)$ then the conclusion is false, since in that case

$$K(\varphi^\lambda_{\alpha,\beta})=e^{d\beta\lambda}K(\varphi)\to0\quad\text{as }\lambda\to-\infty,\tag{2-85}$$

while $J(\varphi^\lambda)$ is away from m, since it is decreasing if $K(\varphi)>0$ and $J(\varphi^\lambda)\nearrow H(\varphi)<m$ if $K(\varphi)<0$.

Proof. We may assume $\varphi\neq0$. Let $j(\lambda)=J(\varphi^\lambda)$ and $n(\lambda)=F(\varphi^\lambda)$, where $\varphi^\lambda_{\alpha,\beta}=\varphi^\lambda$ is the rescaling (1-13). Then $j(0)=J(\varphi)$ and $j'(0)=K(\varphi)$, and (2-18) implies

$$j''\leq(\bar{\mu}+\underline{\mu})j'-\bar{\mu}\underline{\mu}j-\frac{2\alpha\varepsilon}{d+1}n'.\tag{2-86}$$

First we consider the case $K(\varphi)<0$. By Lemma 2.1 together with (2-3), there exists $\lambda_0<0$ such that $j'(\lambda)<0$ for $\lambda_0<\lambda\leq0$ and $j'(\lambda_0)=0$. For $\lambda_0\leq\lambda\leq0$ we have from (2-16),

$$(\bar{\mu}+\underline{\mu})j'-\bar{\mu}\underline{\mu}j\leq\bar{\mu}j'.\tag{2-87}$$

Inserting this in (2-86) and integrating it, we get

$$\int_{\lambda_0}^0 j''(\lambda)\,d\lambda\leq\bar{\mu}\int_{\lambda_0}^0 j'(\lambda)\,d\lambda,\tag{2-88}$$

and hence

$$K(\varphi)=j'(0)\leq\bar{\mu}(j(0)-j(\lambda_0)).\tag{2-89}$$

Since $K(\varphi^{\lambda_0})=0$ and $\varphi^{\lambda_0}\neq0$, we have $j(\lambda_0)=J(\varphi^{\lambda_0})\geq m$. Thus we obtain

$$K(\varphi)\leq-\bar{\mu}(m-J(\varphi)).\tag{2-90}$$

Next we consider the case $K(\varphi)>0$. If

$$(2\bar{\mu}+\underline{\mu})K(\varphi)\geq\bar{\mu}\underline{\mu}J(\varphi)+\frac{2\alpha\varepsilon}{d+1}\mathscr{L}F(\varphi),\tag{2-91}$$

then applying (2-81) to the first term on the right-hand side, and $K=K^Q-\mathscr{L}F$ to the second one, we get

$$\left[2\bar{\mu}+\underline{\mu}+\frac{2\alpha\varepsilon}{d+1}\right]K(\varphi)\geq\frac{\bar{\mu}\underline{\mu}}{2+d}\|\varphi\|^2_{H^1}+\frac{2\alpha\varepsilon}{d+1}K^Q(\varphi),\tag{2-92}$$

and so $K(\varphi)\geq\delta K^Q(\varphi)$ for some $\delta>0$, since $\underline{\mu}>0$ or $\alpha>0$. If (2-91) fails, then

$$(2\bar{\mu}+\underline{\mu})j'<\bar{\mu}\underline{\mu}j+\frac{2\alpha\varepsilon}{d+1}n',\tag{2-93}$$

at $\lambda = 0$, and so from (2-86),

$$j'' < -\bar{\mu} j'. \tag{2-94}$$

Now let λ increase. As long as (2-93) holds and $j' > 0$, we have $j'' < 0$ and so j' decreases and j increases. Also by (2-18) and (2-16) we have

$$n'' \geq (\bar{\mu} + \underline{\mu})n' - \bar{\mu}\underline{\mu}n \geq \bar{\mu}n' \geq \bar{\mu}^2 n > 0. \tag{2-95}$$

Hence (2-93) is preserved until j' reaches 0. It does reach at finite $\lambda_0 > 0$, because the right-hand side of (2-86) is negative and decreasing as long as $j' > 0$. Now integrating (2-94) we obtain

$$K(\varphi) = j'(0) \geq \bar{\mu}(j(\lambda_0) - j(0)) \geq \bar{\mu}(m - J(\varphi)), \tag{2-96}$$

where we used that $J(\varphi^{\lambda_0}) \geq m$ which follows from $K(\varphi^{\lambda_0}) = 0$ and $\varphi^{\lambda_0} \neq 0$. □

3. Blow-up

Here we prove the blow-up part of Theorem 1.1. The idea is essentially due to Payne and Sattinger [1975], but we give a full proof for convenience. We will use that $\mathcal{K}^-$ is stable under the flow.

Assume for a contradiction that a solution u exists for all $t > 0$. (The proof for $t < 0$ is the same.) Let

$$y(t) := \|u(t,x)\|^2_{L^2_x(\mathbb{R}^d)}. \tag{3-1}$$

Multiplying the equation with u, and using (2-82), we get

$$\ddot{y} = 2\|\dot{u}\|^2_{L^2} - 2K_{1,0}(u) \geq (4+c)\|\dot{u}\|^2_{L^2} - 2(2+c)E(u) + c\|u\|^2_{H^1}, \tag{3-2}$$

for some $c > 0$. Sine $u(t) \in \mathcal{K}^-$, Lemma 2.12 implies that there is some positive $\delta \leq -K_{1,0}(u(t))$. Thus for all $t > 0$ we have

$$\ddot{y}(t) \geq 2\delta > 0, \tag{3-3}$$

and so $y(t) = \|u(t)\|^2_{L^2} \to \infty$ as $t \to \infty$. Going back to (3-2), and using Schwarz, we deduce that for large t

$$\ddot{y} \geq (4+c)\|\dot{u}\|^2_{L^2} > \frac{4+c}{4}\frac{\dot{y}^2}{y}, \tag{3-4}$$

therefore

$$(y^{-c/4})_{tt} = -\frac{c}{4} y^{-c/4-2}\left[y\ddot{y} - \frac{4+c}{4}\dot{y}^2\right] < 0, \tag{3-5}$$

which contradicts that $y \to \infty$.

4. Global space-time norm

In this section we introduce Strichartz-type estimates and a perturbation lemma for global space-time bounds of the solution.

The inhomogeneity of the Klein–Gordon equation makes the exponents a bit more complicated than the case of wave or Schrödinger equation. In the H^1 critical case, we get another complication in higher dimensions, due to the fact that we have to estimate the difference of solutions in some Sobolev (or Besov) spaces with positive regularity but the nonlinearity is not twice differentiable.[2] This is not a

[2] The problem is not in the local regularity of the nonlinearity (at $u = 0$), but rather in the global Hölder continuity for f_L.

problem in the subcritical case, where we are allowed to lose small regularity, so that we can estimate the difference in some L^p spaces and then interpolate. This technical issue was solved in the pure critical case in [Nakanishi 1999a] by using space-time norms with exponents away from the admissible region for the standard Strichartz estimate, which was later called "exotic Strichartz estimates" in the Schrödinger case [Tao and Visan 2005].

Here we have a further complication by the presence of lower powers, for which we need the exotic Strichartz for the Klein–Gordon equation. Note that it is not a big trouble in the Schrödinger case (see [Tao et al. 2007]), because the same Strichartz estimate is used both for higher and lower powers. In the Klein–Gordon case, in contrast, we have to use different Strichartz norms, with better regularity for higher powers and with better decay for lower powers. It is easy in the standard Strichartz estimate, where we can freely mix different norms by the duality argument, but this does not work for the exotic Strichartz estimate, which uses exponents away from the duality. Hence we are forced to use a common exponent for different powers, which makes our estimates much more involved. In particular, when we have both the H^1 critical and the L^2 critical powers, we need three steps to close our estimates.

Reduction to a first-order equation. To simplify the notation, we rewrite NLKG as a first-order equation. To any real-valued function $u(t,x)$, we associate a complex-valued[3] function $\vec{u}(t,x)$ thus:

$$\vec{u} = \langle\nabla\rangle u - i\dot{u}, \quad u = \langle\nabla\rangle^{-1}\operatorname{Re}\vec{u}. \tag{4-1}$$

This relation $u \leftrightarrow \vec{u}$ will be assumed for any space-time function u throughout this paper. The free and nonlinear Klein–Gordon equations are given by

$$\begin{aligned} &(\Box+1)u = 0 &&\big(\text{equivalently}, (i\partial_t + \langle\nabla\rangle)\vec{u} = 0\big),\\ &(\Box+1)u = f'(u) &&\big(\text{equivalently}, (i\partial_t + \langle\nabla\rangle)\vec{u} = f'(\langle\nabla\rangle^{-1}\operatorname{Re}\vec{u})\big), \end{aligned} \tag{4-2}$$

and the free energy is given by $E^Q(u) = \|\vec{u}\|_{L^2_x}^2/2$. We set

$$\widetilde{E}(\varphi) := \|\varphi\|_{L^2_x}^2/2 - F(\langle\nabla\rangle^{-1}\operatorname{Re}\varphi), \quad \widetilde{K}_{\alpha,\beta}(\varphi) := K^Q_{\alpha,\beta}(\langle\nabla\rangle^{-1}\varphi) + K^N_{\alpha,\beta}(\langle\nabla\rangle^{-1}\operatorname{Re}\varphi). \tag{4-3}$$

Remark that

$$\widetilde{E}(\vec{u}(t)) = E(u;t), \quad \widetilde{K}(\vec{u}(t)) \ge K(u(t)), \tag{4-4}$$

where the inequality is an equality if and only if $\dot{u}(t) = 0$. The invariant set $\mathcal{K}^+ = \mathcal{K}^+_{\alpha,\beta}$ for $\vec{u}$ is given by

$$\begin{aligned} \widetilde{\mathcal{K}}^+ &:= \{\varphi \in L^2(\mathbb{R}^d) \mid \widetilde{E}(\varphi) < m,\ K(\operatorname{Re}\langle\nabla\rangle^{-1}\varphi) \ge 0\}\\ &= \{\varphi \in L^2(\mathbb{R}^d) \mid \widetilde{E}(\varphi) < m,\ \widetilde{K}(\varphi) \ge 0\}. \end{aligned} \tag{4-5}$$

The second identity is proved as follows. Let $\varphi \in L^2(\mathbb{R}^d)$ satisfy $\widetilde{E}(\varphi) < m$ and $K(\operatorname{Re}\langle\nabla\rangle^{-1}\varphi) < 0$. Let $\psi_1 = \operatorname{Re}\langle\nabla\rangle^{-1}\varphi$ and $\psi_2 = \operatorname{Im}\langle\nabla\rangle^{-1}\varphi$. Then Lemma 2.12 implies that

$$K(\psi_1) \le -\bar{\mu}(m - J(\psi_1)) < -\bar{\mu}\|\psi_2\|_{H^1_x}^2/2 \le -K^Q(\psi_2), \tag{4-6}$$

[3] We do not need the complex structure; we use i purely for notational convenience, and could use vector notation instead, especially if u is originally complex-valued. We chose the complex form rather than the vector one to avoid adding a subscript, for this notation will be applied mostly to sequences.

so $\widetilde{K}(\varphi) = K(\psi_1) + K^Q(\psi_2) < 0$. Hence under the condition $\widetilde{E}(\varphi) < m$, the signs of $K(\psi_1)$ and $\widetilde{K}(\varphi)$ are the same, which proves (4-5).

Strichartz-type estimates and exponents. Here we recall the Strichartz estimate for the free Klein–Gordon equation, introducing some notation for the space-time norms and special exponents.

With any triplet $(b, c, \sigma) \in [0, 1]^2 \times \mathbb{R}$ and any $q \in (0, \infty]$, we associate the following Banach function spaces on $I \times \mathbb{R}^d$ for any interval I:

$$\begin{aligned} [(b, c, \sigma)]_q(I) &:= L_t^{1/b}(I; B^{\sigma}_{1/c,q}(\mathbb{R}^d)), \\ [(b, c, \sigma)]_0(I) &:= L_t^{1/b}(I; L^{1/c}(\mathbb{R}^d)), \\ [(b, c, \sigma)]_q^{\bullet}(I) &:= L_t^{1/b}(I; \dot{B}^{\sigma}_{1/c,q}(\mathbb{R}^d)), \end{aligned} \tag{4-7}$$

where $B^s_{p,q}$ and $\dot{B}^s_{p,q}$ respectively denote the inhomogeneous and homogeneous Besov spaces, and the following characteristic numbers with a parameter $\theta \in [0, 1]$:

$$\begin{aligned} \operatorname{reg}^{\theta}(b, c, \sigma) &:= \sigma - (1 - 2\theta/d)b - d(c - \tfrac{1}{2}), \\ \operatorname{str}^{\theta}(b, c, \sigma) &:= 2b + (d - 1 + \theta)(c - \tfrac{1}{2}), \\ \operatorname{dec}^{\theta}(b, c, \sigma) &:= b + (d - 1 + \theta)(c - \tfrac{1}{2}). \end{aligned} \tag{4-8}$$

The cases $\theta = 0, 1$ correspond respectively to the wave and the Klein–Gordon equations. $\operatorname{reg}^{\theta}$ indicates the regularity of the space, while $\operatorname{str}^{\theta}$ and $\operatorname{dec}^{\theta}$ indicate the space-time decay, corresponding respectively to the Strichartz and the $L^p - L^q$ decay estimates. We denote the regularity change and the duality in $H^{s-1/2}$ (here $-\frac{1}{2}$ takes account of one regularity gain in the wave equation) respectively by

$$(b, c, \sigma)^s := (b, c, s), \quad (b, c, \sigma)^{*(s)} := (1 - b, 1 - c, -\sigma + 2s - 1). \tag{4-9}$$

Given a real number s, we say that $Z = (Z_1, Z_2, Z_3)$ is Strichartz s-admissible if for some $\theta \in [0, 1]$ we have

$$0 \le Z_1 \le \tfrac{1}{2}, \quad 0 \le Z_2 < \tfrac{1}{2}, \quad \operatorname{reg}^{\theta}(Z) \le s, \quad \operatorname{str}^{\theta}(Z) \le 0. \tag{4-10}$$

We avoid the endpoint $Z_2 = \frac{1}{2}$ to mix different θ's. We now state the Strichartz estimates:

Lemma 4.1 (see [Brenner 1984; Ginibre and Velo 1985a; Machihara et al. 2002]). *For any $s \in \mathbb{R}$, let Z and T be s-admissible. Then for any space-time function $u(t, x)$, any interval $I \subset \mathbb{R}$, and any $t_0 \in I$, we have*

$$\|u\|_{[Z]_2(I)} \lesssim \|u(t_0)\|_{H^s} + \|\dot{u}(t_0)\|_{H^{s-1}} + \|\ddot{u} - \Delta u + u\|_{[T^{*(s)}]_2(I)}, \tag{4-11}$$

where the implicit constant does not depend on I or t_0.

The "exotic Strichartz estimate" is given for the Klein–Gordon equation by

Lemma 4.2. *Let $Z, T \in \mathbb{R}^3$ satisfy for some $\theta \in [0, 1]$*

$$\begin{aligned} &\operatorname{reg}^{\theta}(Z) \le \operatorname{reg}^{\theta}(T) + 2, \quad \operatorname{str}^{\theta}(Z) \le \operatorname{str}^{\theta}(T) - 2, \quad 0 < Z_1, T_1 < 1, \\ &\operatorname{dec}^{\theta}(Z) < 0 < \operatorname{dec}^{\theta}(T) - 1, \quad 0 < \frac{1}{2} - Z_2, T_2 - \frac{1}{2} < \frac{1}{d-1+\theta}. \end{aligned} \tag{4-12}$$

Then, for any interval $I \subset \mathbb{R}$, $t_0 \in I$, *and* $u(t,x)$ *satisfying* $u(t_0) = \dot u(t_0) = 0$,

$$\|u\|_{[Z]_2(I)} \lesssim \|\ddot u - \Delta u + u\|_{[T]_2(I)}. \tag{4-13}$$

Proof. The wave case $\theta = 0$ was essentially proved in [Nakanishi 1999a, Lemma 7.4], where the borderline case $\mathrm{str}^0(Z) = \mathrm{str}^0(T) - 2$ was excluded for the real interpolation to improve the Besov exponent 2. Here we discard that improvement, restoring the borderline case, which is needed for the lower critical power $p_1 = 4/d$.

The proof is rather immediate from the standard Strichartz estimate and the L^p decay estimate. Indeed, if $\mathrm{str}^\theta(Z) = 0 = \mathrm{str}^\theta(T) - 2$ and $\mathrm{reg}^\theta(Z) = \mathrm{reg}^\theta(T) + 2$, then the above estimate is nothing but Strichartz. If moreover $Z_2 + T_2 = 1$, then the estimate directly follows from the L^p decay and the Hardy–Littlewood–Sobolev inequality

$$\begin{aligned}\Big\| \int_{t_0}^t \langle\nabla\rangle^{-1} e^{\pm i(t-s)\langle\nabla\rangle} h(s)\, ds \Big\|_{[Z]_2(I)} &\lesssim \Big\| \int_{t_0}^t |t-s|^{-2Z_1} \|h(s)\|_{B^{T_3}_{1/T_2,2}}\, ds \Big\|_{L^{1/T_1}(I)} \\ &\lesssim \|h\|_{[T]_2(I)}.\end{aligned} \tag{4-14}$$

This estimate can be translated in the time and the regularity exponents as

$$Z \mapsto Z' = Z + (b, 0, s), \quad T \mapsto T' = T + (b, 0, s) \tag{4-15}$$

for any $s \in \mathbb{R}$ and $b \in (-1/2, 1/2)$, as long as $0 < Z_1', T_1' < 1$. By the complex interpolation for those estimates and the standard Strichartz estimate, we obtain the desired estimate in the case $\mathrm{str}^\theta(Z) = \mathrm{str}^\theta(T) - 2$ and $\mathrm{reg}^\theta(Z) = \mathrm{reg}^\theta(T) + 2$. It is extended to the remaining cases (with inequality in these relations) by the Sobolev embedding. □

The following interpolation is convenient for switching from some exponents to others:

Lemma 4.3. *Let* $Z, A, B, C \in [0,1] \times \mathbb{R}$ *and* $\theta \in [0,1]$. *Assume that* $A_1 < Z_1 < B_1$ *and that either*

(1) $\min(\mathrm{str}^\theta(A), \mathrm{str}^\theta(B), \mathrm{str}^\theta(C)) \ge \mathrm{str}^\theta(Z)$ *and* $\min(\mathrm{reg}^\theta(A), \mathrm{reg}^\theta(B)) > \mathrm{reg}^\theta(Z)$, *or*

(2) $\min(\mathrm{str}^\theta(A), \mathrm{str}^\theta(B)) > \mathrm{str}^\theta(Z)$ *and* $\min(\mathrm{reg}^\theta(A), \mathrm{reg}^\theta(B), \mathrm{reg}^\theta(C)) \ge \mathrm{reg}^\theta(Z)$.

Then there exist $\alpha, \beta, \gamma \in (0,1)$ *such that* $\alpha + \beta + \gamma = 1$ *and that, for all* $q \in (0, \infty]$, *we have the interpolation inequality*

$$\|u\|_{[Z]_q} \lesssim \|u\|^\alpha_{[A]_\infty} \|u\|^\beta_{[B]_\infty} \|u\|^\gamma_{[C]_\infty}. \tag{4-16}$$

Proof. Since $A_1 < Z_1 < B_1$, for any $0 < \theta_2 \ll 1$ there exists $\theta_1 \in (0,1)$ such that

$$(1-\theta_2)((1-\theta_1)A_1 + \theta_1 B_1) + \theta_2 C_1 = Z_1. \tag{4-17}$$

Let $\widetilde Z := (1-\theta_2)((1-\theta_1)A + \theta_1 B) + \theta_2 C$. Then from the assumption we have

$$\mathrm{str}^\theta(\widetilde Z) \ge \mathrm{str}^\theta(Z), \quad \mathrm{reg}^\theta(\widetilde Z) \ge \mathrm{reg}^\theta(Z), \tag{4-18}$$

which imply $\widetilde Z_2 \ge Z_2$ and $\widetilde Z_3 - d\widetilde Z_2 \ge Z_3 - dZ_2$, and so we have the Sobolev embedding $[\widetilde Z]_q \subset [Z]_q$. In the first case, we have $\mathrm{reg}^\theta(\widetilde Z) > \mathrm{reg}^\theta(Z)$ and so

$$\big[[[A]_\infty, [B]_\infty]_{\theta_1}, [C]_\infty\big]_{\theta_2} = [\widetilde Z]_\infty \subset [Z]_q. \tag{4-19}$$

The desired inequality follows from that for the complex interpolation.

It remains to prove the result under condition (2). By the real interpolation in the Besov space in x and Hölder in t, we have for all $0 < \delta \ll 1$,

$$\|u\|_{[Z]_q} \lesssim \|u\|_{[Z+]_\infty}^{1/2} \|u\|_{[Z-]_\infty}^{1/2}, \quad Z^\pm := Z \pm \delta(1, 0, 1-2\theta/d). \tag{4-20}$$

Let $0 < \varepsilon \ll 1$ satisfy $\varepsilon(B_1 - A_1)(1-\theta_2) = \delta$ and

$$\widetilde{Z}^\pm := (1-\theta_2)((1-\theta_1 \mp \varepsilon)A + (\theta_1 \pm \varepsilon)B) + \theta_2 C. \tag{4-21}$$

Then from the assumption and the definition of $Z^\pm$ and ε, we have

$$\operatorname{str}^\theta(\widetilde{Z}^\pm) > \operatorname{str}^\theta(Z^\pm), \quad \operatorname{reg}^\theta(\widetilde{Z}^\pm) \geq \operatorname{reg}^\theta(Z^\pm) = \operatorname{reg}^\theta(Z), \tag{4-22}$$

when $\varepsilon > 0$ is small. Hence we have the Sobolev embedding

$$\big[[[A]_\infty, [B]_\infty]_{\theta_1 \pm \varepsilon}, [C]_\infty\big]_{\theta_2} = [\widetilde{Z}^\pm]_\infty \subset [Z^\pm]_\infty, \tag{4-23}$$

where the left-hand side is a nested complex interpolation space. Now the conclusion follows from the interpolation inequality. □

Global perturbation of Strichartz norms. Now we fix a few particular exponents. Define H, W, K by

$$H := \Big(0, \frac{1}{2}, 1\Big), \quad W := \Big(\frac{d-1}{2(d+1)}, W_1, \frac{1}{2}\Big), \quad K := \Big(\frac{d}{2(d+2)}, K_1, \frac{1}{2}\Big). \tag{4-24}$$

Then $[H]_2 = L_t^\infty H_x^1$ is the energy space, while W and K are 1-admissible, diagonal and boundary exponents respectively for the wave ($\theta = 0$) and the Klein–Gordon ($\theta = 1$) equations:

$$\begin{aligned} 1 &= \operatorname{reg}^0(H) = \operatorname{reg}^1(H) = \operatorname{reg}^0(W) = \operatorname{reg}^1(K), \\ 0 &= \operatorname{str}^0(H) = \operatorname{str}^1(H) = \operatorname{str}^0(W) = \operatorname{str}^1(K). \end{aligned} \tag{4-25}$$

Let $eq(u)$ denote the left-hand side of NLKG:

$$eq(u) := u_{tt} - \Delta u + u - f'(u). \tag{4-26}$$

Recall the convention $u \leftrightarrow \vec{u}$ (page 427) to switch to first-order equations. We will treat the H^1 critical case (1-28) together with the subcritical case. Since $f_S(u)$ is for small $|u|$ and $f_L(u)$ for large $|u|$, we may freely lower p_1 in (1-25) and raise p_2 in (1-26). Hence we assume (1-25) with

$$2_\star - 2 = \frac{4}{d} < p_1 < \frac{4(d+1)}{(d+2)(d-1)}, \tag{4-27}$$

and we assume either $d = 1$, (1-29), or (1-26), with

$$\frac{4(d+1)}{d^2-d-1} < p_2 \leq 2^\star - 2. \tag{4-28}$$

Before the main perturbation lemma, we see that $[H]_2 \cap [W]_2 \cap [K]_2$ is enough to bound the full Strichartz norms of the solutions.

Lemma 4.4. *Assume that f satisfies* (1-36). *Let Z, T and U be* 1*-admissible. In the* 2*D exponential case* (1-29), *let* $\Theta \in (0,1)$. *Then there exist a constant $C_1 > 0$ and a continuous function $C_2 : (0,\infty) \to (0,\infty)$ such that for any interval I, any $t_0 \in I$ and any $w(t,x)$, we have*

$$\|w\|_{[Z]_2(I)} \le C_1\|\vec{w}(t_0)\|_{L^2_x} + C_1\|eq(w)\|_{([T^{*(1)}]_2+[U^{*(1)}]_2)(I)} + C_2(\|w\|_{([H]_2\cap[W]_2\cap[K]_2)(I)}), \tag{4-29}$$

provided, *in the exponential case*, *that*

$$\sup_{t\in I}\kappa_0\|\nabla w\|^2_{L^2_x} \le 4\pi\Theta. \tag{4-30}$$

We remark that (4-30) is needed only in the exponential case.

Proof. We may assume $\Theta > \frac{1}{2}$ without losing any generality. We introduce the new exponents $M^\sharp$ and X by

$$M^\sharp := \frac{2}{p_2(d+1)}(1,1,0), \quad X := (\nu, 0, \nu-\nu^2), \tag{4-31}$$

with some $\nu \in (0, 1/10)$ satisfying $\Theta < (1-\nu)^2$, where $M^\sharp$ is used only if $d \ge 2$ and X only in the exponential case. In either case we have

$$0 > \mathrm{str}^0(M^\sharp), \quad 0 > \mathrm{str}^0(X), \quad 1 \ge \mathrm{reg}^0(M^\sharp), \quad 1 > \mathrm{reg}^0(X), \quad 0 < M^\sharp_1, X_1 < W_1. \tag{4-32}$$

Hence by Lemma 4.3(1), we have

$$\|w\|_{[M^\sharp]_2(I)} + \|w\|_{[X]_2(I)} \lesssim \|w\|_{([H]_2\cap[W]_2\cap[K]_2)(I)}. \tag{4-33}$$

The Strichartz estimate gives

$$\|w\|_{[Z]_2(I)} \lesssim \|\vec{w}(t_0)\|_{L^2_x} + \|eq(w)\|_{([T^{*(1)}]_2+[U^{*(1)}]_2)(I)} + \|f'(w)\|_{([K^{*(1)}]_2+[W^{*(1)}]_2+L^1_tL^2_x)(I)}. \tag{4-34}$$

By the standard nonlinear estimate we have

$$\|f'_S(w)\|_{[K^{*(1)}]_2(I)} \lesssim \|w\|_{[K]_2(I)}\|w\|^{4/d}_{[K]_0(I)}, \tag{4-35}$$

and in the subcritical/critical cases

$$\|f'_L(w)\|_{[W^{*(1)}]_2(I)} \lesssim \|w\|_{[W]_2(I)}\|w\|^{p_2}_{[M^\sharp]_0(I)}. \tag{4-36}$$

In the exponential case, there are $\kappa > \kappa_0$ and $\mu > 0$ such that

$$\sup_{t\in I}\kappa\|w\|^2_{H^1_\mu} \le 4\pi\Theta', \tag{4-37}$$

where $\Theta' := \dfrac{1+\Theta}{2} < 1$ and

$$\|\varphi\|_{H^1_\mu} := \|\nabla\varphi\|^2_{L^2_x} + \mu\|\varphi\|^2_{L^2_x}. \tag{4-38}$$

Then we have

$$\|f'_L(w)\|_{L^2_x} \lesssim \||w|(e^{\kappa|w|^2}-1)\|_{L^2_x} \lesssim \|w\|_{L^\infty_x}\|e^{\kappa|w|^2}-1\|^{1/2}_{L^1_x}\|e^{\kappa|w|^2}\|^{1/2}_{L^\infty_x}, \tag{4-39}$$

where the second factor is bounded by Trudinger–Moser:

$$\|e^{\kappa|w|^2}-1\|_{L^1_x} \lesssim \|w\|_{L^2}^2/(1-\Theta'), \tag{4-40}$$

and the third factor is bounded by the following log-interpolation inequality [Ibrahim et al. 2007, Theorem 1.3]: for any $\alpha \in (0,1)$, $\lambda > 1/(2\pi\alpha)$ and $\mu > 0$, there is $C > 0$ such that

$$\|\varphi\|_{L^\infty(\mathbb{R}^2)}^2 \le \lambda\|\varphi\|_{H^1_\mu(\mathbb{R}^2)}^2\big[C+\log(1+\|\varphi\|_{C^\alpha(\mathbb{R}^2)}/\|\varphi\|_{H^1_\mu(\mathbb{R}^2)})\big], \tag{4-41}$$

for any $\varphi \in H^1 \cap C^\alpha(\mathbb{R}^2)$, where $C^\alpha = B^\alpha_{\infty,\infty}$ denotes the Hölder space. Plugging this with $\alpha := \nu-\nu^2$ into the exponential, we get

$$\|e^{\kappa|w|^2}\|_{L^\infty_x} \lesssim \big(1+\|w\|_{C^\alpha_x}/\|w\|_{H^1_\mu}\big)^{\lambda\kappa\|w\|^2_{H^1_\mu}} \lesssim \big(1+\kappa\|w\|^2_{C^\alpha_x}/\Theta'\big)^{2\pi\lambda\Theta'}, \tag{4-42}$$

where $\lambda > 0$ is chosen so that

$$1 < 2\pi\lambda\alpha, \quad (2\pi\lambda\Theta'+1)\nu = 1. \tag{4-43}$$

Since f_L vanishes for small $|u|$, we may assume $\|w\|_{C^\alpha_x} \gtrsim \|w\|_{L^\infty_x} \gtrsim 1$. Hence

$$\|e^{\kappa|w|^2}\|_{L^\infty_x} \lesssim \|w\|_{C^\alpha_x}^{4\pi\lambda\Theta'} = \|w\|_{C^\alpha_x}^{2(1/\nu-1)}, \tag{4-44}$$

and plugging this into (4-39), we get

$$\|f_L'(w)\|_{L^1_tL^2_x} \lesssim \|w\|_{L^{1/\nu}_tL^\infty_x}\|w\|_{L^\infty_tL^2_x}\|w\|^{1/\nu-1}_{L^{1/\nu}_tC^\alpha_x} \lesssim \|w\|^{1/\nu}_{[X]_2}\|w\|_{[H]_2}, \tag{4-45}$$

which concludes the proof. □

Lemma 4.5. *Assume that f satisfies* (1-36). *Let Z, T, U and V be* 1*-admissible and* $\mathrm{reg}^0(V) = 1$. *In the exponential case* (1-29), *let $\Theta \in (0,1)$. Then there are continuous functions $\varepsilon_0, C_0 : (0,\infty)^2 \to (0,\infty)$ such that the following holds*: *Let $I \subset \mathbb{R}$ be an interval, $t_0 \in I$ and $\vec{u}, \vec{w} \in C(I; L^2(\mathbb{R}^d))$. Let $\vec{\gamma}_0 = e^{i\langle\nabla\rangle(t-t_0)}(\vec{u}-\vec{w})(t_0)$ and assume that for some $A, B > 0$ we have*

$$\|\vec{u}\|_{L^\infty_t(I;L^2_x)} + \|\vec{w}\|_{L^\infty_t(I;L^2_x)} \le A, \tag{4-46}$$

$$\|w\|_{[W]_2(I)\cap[K]_2(I)} \le B, \tag{4-47}$$

$$\|(eq(u), eq(w))\|_{([T^{*(1)}]_2+[U^{*(1)}]_2)(I)} + \|\gamma_0\|_{[V]_\infty(I)} \le \varepsilon_0(A,B), \tag{4-48}$$

and in the exponential case,

$$\sup_{t\in I}\kappa_0\max(\|\nabla u\|^2_{L^2_x}, \|\nabla w\|^2_{L^2_x}) \le 4\pi\Theta. \tag{4-49}$$

Then we have

$$\|u\|_{[Z]_2(I)} \le C_0(A,B). \tag{4-50}$$

Remark 4.6. (4-49) is needed only in the exponential case. The lemma remains valid in the lower critical case $p_1 = 4/d = 2_\star - 2$, if we assume in addition that

$$\|\gamma_0\|_{[K]_0(I)} \le \varepsilon_0(A,B). \tag{4-51}$$

We will indicate the necessary modifications in the proof.

Proof of Lemma 4.5. We restrict p_1, p_2 as in (4-27) and (4-28), without losing any generality. In the following, $C(\cdot, \dots)$ denotes arbitrary positive constants which may depend continuously on the indicated parameters. Let $\delta \in (0,1)$ be a fixed small number, whose smallness will be specified by the following arguments. Let

$$e := eq(u) - eq(w), \quad \gamma := u - w. \tag{4-52}$$

Then we have the equation for the difference

$$\ddot{\gamma} - \Delta\gamma + \gamma = f'(w+\gamma) - f'(w) - e, \quad \vec{\gamma}(t_0) = \vec{\gamma}_0(t_0). \tag{4-53}$$

First note that by Lemma 4.4, we have the full Strichartz norms on w.

Next we estimate the difference $u - w$ in the easier case $d \le 4$. We define new exponents S, L and a space $\mathscr{X}$ by

$$\begin{gathered}[S]_0 := L_t^{p_1+1} L_x^{2(p_1+1)}, \quad [L]_0 := L_t^{p_2+1} L_x^{2(p_2+1)}, \\ \mathscr{X} := \begin{cases} [S]_0 & (d=1) \\ [S]_0 \cap [X]_2 & (1\text{-}29), \\ [S]_0 \cap [L]_0 & (\text{otherwise}). \end{cases}\end{gathered} \tag{4-54}$$

Thanks to the restrictions (4-27) and (4-28), we have

$$0 > \operatorname{str}^1(S), \quad 0 > \operatorname{str}^0(L), \quad 1 > \operatorname{reg}^1(S), \quad 1 > \operatorname{reg}^0(L). \tag{4-55}$$

Hence by Lemma 4.3(2) with $C := V$, we get for some $\theta_1, \theta_2 \in (0,1)$,

$$\|\gamma_0\|_{\mathscr{X}(I)} \lesssim A^{1-\theta_1}\varepsilon_0^{\theta_1} + A^{1-\theta_2}\varepsilon_0^{\theta_2}. \tag{4-56}$$

If $p_1 \to 4/d$, then $\operatorname{str}^0(S) \to 0$, and we would need the smallness in $[K]_0(I)$.

Since $w \in \mathscr{X}(I)$ by Lemma 4.4, there exists a partition of the right half of I:

$$t_0 < t_1 < \dots < t_n, \quad I_j = (t_j, t_{j+1}), \quad I \cap (t_0, \infty) = (t_0, t_n) \tag{4-57}$$

such that $n \le C(A, B, \delta)$ and

$$\|w\|_{\mathscr{X}(I_j)} \le \delta \quad (j = 0, \dots, n-1). \tag{4-58}$$

We omit the estimate on $I \cap (-\infty, t_0)$ since it is the same by symmetry.

Let γ_j be the free solution defined by

$$\vec{\gamma}_j := e^{i\langle\nabla\rangle(t-t_j)}\vec{\gamma}(t_j). \tag{4-59}$$

Then the Strichartz estimate applied to the equations of γ and γ_{j+1} implies

$$\|\gamma - \gamma_j\|_{\mathscr{X}(I_j)} + \|\gamma_{j+1} - \gamma_j\|_{\mathscr{X}(\mathbb{R})} \lesssim \|f'(w+\gamma) - f'(w)\|_{L_t^1 L_x^2(I_j)} + \|e\|_{([U^{*(1)}]_2 + [T^{*(1)}]_2)(I_j)}. \tag{4-60}$$

The nonlinear difference is estimated as follows. For smaller $|u|$, we have by Hölder

$$\|f_S'(w+\gamma) - f_S'(w)\|_{L_t^1 L_x^2} \lesssim \|(w,\gamma)\|_{[S]_0}^{p_1} \|\gamma\|_{[S]_0}, \tag{4-61}$$

and for larger $|u|$ for $d \geq 2$ in the subcritical/critical cases,

$$\|f_L'(w+\gamma) - f_L'(w)\|_{L_t^1 L_x^2} \lesssim \|(w,\gamma)\|_{[L]_0}^{p_2} \|\gamma\|_{[L]_0}. \tag{4-62}$$

If $d = 1$, let $C(\nu) = \sup_{|u| \leq \nu} |f_L''(u)|/|u|^{p_1}$. Then we have

$$\begin{aligned}\|f_L'(w+\gamma) - f_L'(w)\|_{L_t^1 L_x^2} &\lesssim C(\|w\|_{L_{t,x}^\infty} + \|\gamma\|_{L_{t,x}^\infty}) \|(w,\gamma)\|_{[S]_0}^{p_1} \|\gamma\|_{[S]_0} \\ &\lesssim C(\|(w,\gamma)\|_{L_t^\infty H_x^1}) \|(w,\gamma)\|_{[S]_0}^{p_1} \|\gamma\|_{[S]_0}.\end{aligned} \tag{4-63}$$

In the exponential case, there exist $\kappa > \kappa_0$ and $\mu > 0$ such that (4-37). Let $w_\theta = w + \theta\gamma = (1-\theta)w + \theta u$ for $\theta \in [0,1]$. Then we have

$$\kappa \|w_\theta\|_{H_\mu^1}^2 \leq 4\pi\Theta',$$

where $\Theta' = \dfrac{1+\Theta}{2}$ and H_μ^1 is defined in (4-38). In the same way as for (4-45), we obtain

$$\begin{aligned}\|f_L'(w+\gamma) - f_L'(w)\|_{L_t^1 L_x^2} \leq \int_0^1 \|f_L''(w_\theta)\gamma\|_{L_t^1 L_x^2} d\theta &\lesssim \sup_{\theta \in [0,1]} \|w_\theta\|_{[H]_2} \|w_\theta\|_{[X]_2}^{1/\nu - 1} \|\gamma\|_{[X]_2} \\ &\lesssim A \|(w,\gamma)\|_{[X]_2}^{1/\nu-1} \|\gamma\|_{[X]_2}.\end{aligned} \tag{4-64}$$

Thus in all cases, assuming

$$\|\gamma\|_{\mathscr{X}(I_j)} \leq \delta \ll 1 \quad (j = 0, \dots, n-1), \tag{4-65}$$

where the smallness depends on A (and Θ), we get

$$\|\gamma\|_{\mathscr{X}(I_j)} + \|\gamma_{j+1}\|_{\mathscr{X}(t_{j+1},t_n)} \leq C\|\gamma_j\|_{\mathscr{X}(t_j,t_n)} + \varepsilon_0, \tag{4-66}$$

for some absolute constant $C \geq 2$. Then by (4-56) and iteration in j we get

$$\|\gamma\|_{\mathscr{X}(I)} \lesssim (2C)^n (A^{1-\theta_1}\varepsilon_0^{\theta_1} + A^{1-\theta_2}\varepsilon_0^{\theta_2}) \leq C(A,B)(\varepsilon_0^{\theta_1} + \varepsilon_0^{\theta_2}). \tag{4-67}$$

Choosing $\varepsilon_0(A,B)$ sufficiently small, we can make the last bound much smaller than δ, and thus the assumption (4-65) is justified by continuity in t and induction on j. Then repeating the estimate (4-60) once more, we can estimate the full Strichartz norms on γ, which implies also the bound on u.

Next we estimate the difference $u - w$ in the harder case $d \geq 5$, where we need the new exponents $\widetilde{M}$, M, $\widetilde{N}$, N, R, Q, P, and Y defined by

$$\begin{aligned}
M &= \frac{2}{d+1}\left[\frac{1}{p_2}(1+d,0,0) - \frac{d-2}{4}(d,-1,0)\right], \\
\widetilde{N} &= \frac{2}{d+1}\left[\left(\frac{1}{2},\frac{d-1}{4},1\right) + \left(1 - \frac{d-2}{4}p_2\right)(-d,1,0)\right], \\
\widetilde{M} &= M + \frac{2}{p_2(d+1)}(0,1/d,1), \quad N = \widetilde{N} - \frac{2}{d+1}(0,1/d,1), \\
Q &= \frac{(1,2,2)}{p_1(d+1)}, \quad P = \frac{(4,d-1,4)}{2(d+1)}, \quad Y = \frac{(6,d+3,4)}{2(d+1)}, \\
R &= \left(\frac{(d+4)}{2(d+2)(p_1+1)}, R_1, \frac{1}{2}\right).
\end{aligned} \tag{4-68}$$

In the case $p_2 > 1$, we need another exponent

$$\widehat{M} := \widetilde{M} + \frac{2(p_2-1)}{p_2(d+1)}(0, 1/d, 1), \tag{4-69}$$

and if $p_2 \le 1$ then we put $\widehat{M} = \widetilde{M}$. Note that $p_1 < 1$ under (4-27) for $d \le 5$. Then we have the sharp Sobolev embedding

$$[\widehat{M}]_q \subset [\widetilde{M}]_q \subset [M]_q, \quad [\widetilde{N}]_q \subset [N]_q, \tag{4-70}$$

and nonlinear and interpolation relations

$$R + p_1 R^0 = K^{*(1)}, \quad R = (1-\alpha)W + \alpha K, \quad M^\sharp = (1-\beta)W^0 + \beta R^0, \tag{4-71}$$

for some $\alpha, \beta \in (0,1)$, thanks to (4-27) and (4-28). Y is a non-admissible exponent satisfying

$$Y = \widetilde{N} + p_2 M = N + p_2 \widetilde{M} = P + p_1 Q^0 = P^0 + p_1 Q, \tag{4-72}$$

where the second and the last identities follow from $P_3 = p_1 Q_3$, $\widetilde{N}_3 = p_2 \widetilde{M}_3$, and the above sharp embeddings. If $p_2 > 1$, we have in addition

$$Y = N + \widehat{M} + (p_2 - 1)M. \tag{4-73}$$

These exponents satisfy (when $d \ge 5$)

$$\begin{gathered} 1 = \operatorname{reg}^0(\widetilde{N}) = -\operatorname{reg}^0(Y) \ge \operatorname{reg}^0(\widehat{M}), \quad 1 > \operatorname{reg}^1(Q), \operatorname{reg}^1(P), -\operatorname{reg}^1(Y), \\ 0 > \operatorname{str}^0(\widehat{M}), \operatorname{str}^0(\widetilde{N}), \operatorname{str}^1(Q), \operatorname{str}^1(P), \\ \operatorname{str}^0(\widetilde{N}) \le \operatorname{str}^0(Y) - 2, \quad \operatorname{str}^1(P) = \operatorname{str}^1(Y) - 2, \\ 0 \le \widehat{M}_1, \widehat{M}_2, Q_1, Q_2, R_1 < \tfrac{1}{2}, \quad 1 < \operatorname{dec}^0(Y), \operatorname{dec}^1(Y), \\ Y_2 < \frac{1}{2} + \frac{1}{d}, \quad \widetilde{N}_2 > \frac{1}{2} - \frac{1}{d-1}, \quad P_2 > \frac{1}{2} - \frac{1}{d}. \end{gathered} \tag{4-74}$$

Moreover, $\operatorname{reg}^0(\widehat{M}) = 1$ only if $p_2 = 2^\star - 2 = 4/(d-2)$. Lemma 4.3(1) implies that

$$\|w\|_{([Q]_{2p_1} \cap [\widehat{M}]_2 \cap [\widetilde{M}]_{2p_2})(I)} \lesssim \|w\|_{([H]_2 \cap [K]_2 \cap [W]_2)(I)} \lesssim A + B. \tag{4-75}$$

As before, we divide $I \cap (t_0, \infty)$ into $t_0 < \cdots < t_n$, $n \le C(A,B)$ such that

$$\|w\|_{([Q]_{2p_1} \cap [\widehat{M}]_2 \cap [\widetilde{M}]_{2p_2} \cap [K]_2 \cap [W]_2)(I_j)} \le \delta \ll 1 \quad (j = 0, \dots, n-1). \tag{4-76}$$

We also introduce the following spaces:

$$\begin{aligned} &\mathcal{Y}_0 := [W]_0 \cap [R]_0, \quad \widetilde{\mathcal{Y}} := [\widetilde{N}]_2 \cap [P]_2, \quad \mathcal{Y} := [W]_2 \cap [K]_2, \\ &\mathcal{Y}_0^* := [W^{*(1)}]_0 + [K^{*(1)}]_0, \quad \mathcal{Y}^* := [W^{*(1)}]_2 + [K^{*(1)}]_2. \end{aligned} \tag{4-77}$$

Our proof for $d \ge 5$ consists of three steps:

(1) We estimate γ in $\mathcal{Y}_0$, assuming it is bounded in some norm similar to (4-76). Here we can use the standard Strichartz because the estimates do not contain spatial derivative.

(2) We estimate γ in $\widetilde{\mathcal{Y}}$, under the same assumption on γ. Here we use the exotic Strichartz.

(3) We estimate u in $\mathcal{Y}$ by using the bounds in $[\widetilde{N}]_2 \cap [R]_0$. The assumption in the previous steps is justified once we get a better bound.

Actually we could skip the first step, by using interpolation in the last step to bound $[R]_0$ by the other norms. However, if $p_1 = 4/d$ the lower critical power, then $R = K$ and the first step becomes necessary.

Assuming that

$$\|\gamma\|_{([Q]_{2p_1}\cap[\widehat{M}]_{2p_2}\cap[R]_0\cap[M^\sharp]_0)(I_j)} \le \delta \quad (j = 0, \dots, n-1), \tag{4-78}$$

we have by Strichartz and Hölder (since W^0 and R^0 are $\frac{1}{2}$-admissible)

$$\begin{aligned}\|\gamma-\gamma_j\|_{\mathcal{Y}_0(I_j)} + \|\gamma_{j+1}-\gamma_j\|_{\mathcal{Y}_0(\mathbb{R})} &\lesssim \|f'(w+\gamma) - f'(w)\|_{\mathcal{Y}_0^*(I_j)} + \|e\|_{\mathcal{Y}^*(I_j)} \\ &\lesssim \|(w,\gamma)\|_{[R]_0(I_j)}^{p_1}\|\gamma\|_{[R]_0(I_j)} + \|(w,\gamma)\|_{[M^\sharp]_0(I_j)}^{p_2}\|\gamma\|_{[W]_0(I_j)} + \varepsilon_0 \\ &\lesssim \delta^{p_1}\|\gamma\|_{\mathcal{Y}_0(I_j)} + \varepsilon_0,\end{aligned} \tag{4-79}$$

where we used (4-76) and (4-78). By Lemma 4.3(2), we have

$$\|\gamma_0\|_{\mathcal{Y}_0(I)} \lesssim A^{1-\theta_3}\varepsilon_0^{\theta_3} + A^{1-\theta_4}\varepsilon_0^{\theta_4}, \tag{4-80}$$

for some $\theta_3, \theta_4 \in (0,1)$. Note that $\operatorname{str}^1(R) \to 0$ as $p_1 \to 4/d$, hence in the lower critical case we would need γ_0 to be small in $[K]_0$. By the same argument as for (4-67), we obtain

$$\|\gamma\|_{\mathcal{Y}_0(I)} \le C(A,B)(\varepsilon_0^{\theta_3} + \varepsilon_0^{\theta_4}) \ll \delta. \tag{4-81}$$

Next, still assuming (4-78), we have by the exotic Strichartz estimate,

$$\|\gamma-\gamma_j\|_{\widetilde{\mathcal{Y}}(I_j)} + \|\gamma_{j+1}-\gamma_j\|_{\widetilde{\mathcal{Y}}(\mathbb{R})} \lesssim \|f'(w+\gamma) - f'(w)\|_{[Y]_2(I_j)} + \|e\|_{\mathcal{Y}^*(I_j)}, \tag{4-82}$$

where the nonlinear difference is estimated by

$$\begin{aligned}&\|f_L'(w+\gamma) - f_L'(w)\|_{[Y]_2} \\ &\quad\lesssim \|(w,\gamma)\|_{[M]_0}^{p_2}\|\gamma\|_{[\widetilde{N}]_2} + \|(w,\gamma)\|_{[\widetilde{M}]_{2p_2}}^{p_2}\|\gamma\|_{[N]_0} + \|(w,\gamma)\|_{[M]_0}^{p_2-1}\|(w,\gamma)\|_{[\widehat{M}]_2}\|\gamma\|_{[N]_0},\end{aligned} \tag{4-83}$$

where the last term is for $p_2 > 1$ while the second last is for $p_2 \le 1$, and similarly

$$\|f_S'(w+\gamma) - f_S'(w)\|_{[Y]_2} \lesssim \|(w,\gamma)\|_{[Q]_0}^{p_1}\|\gamma\|_{[P]_2} + \|(w,\gamma)\|_{[Q]_{2p_1}}^{p_1}\|\gamma\|_{[P]_0}. \tag{4-84}$$

Thus we obtain

$$\|\gamma-\gamma_j\|_{\widetilde{\mathcal{Y}}(I_j)} + \|\gamma_{j+1}-\gamma_j\|_{\widetilde{\mathcal{Y}}(\mathbb{R})} \lesssim \delta^{p_1}\|\gamma\|_{\widetilde{\mathcal{Y}}(I_j)} + \varepsilon_0, \tag{4-85}$$

where we used (4-76), (4-78), and the following embeddings in x

$$[Q]_{2p_1} \subset [Q]_0, \quad [P]_2 \subset [P]_0, \quad [\widehat{M}]_2 + [\widetilde{M}]_{2p_2} \subset [M]_0, \quad [\widetilde{N}]_2 \subset [N]_0. \tag{4-86}$$

By Lemma 4.3 and Strichartz, we have

$$\begin{aligned}\|\gamma_0\|_{[\widetilde{N}]_2(I)} &\lesssim \|\gamma_0\|_{[H]_2(I)\cap[W]_2(I)}^{1-\theta_5}\|\gamma_0\|_{[M]_0(I)}^{\theta_5} \lesssim A^{1-\theta_5}\varepsilon_0^{\theta_5}, \\ \|\gamma_0\|_{[P]_2(I)} &\lesssim \|\gamma_0\|_{[H]_2(I)\cap[K]_2(I)}^{1-\theta_6}\|\gamma_0\|_{[M]_0(I)}^{\theta_6} \lesssim A^{1-\theta_6}\varepsilon_0^{\theta_6},\end{aligned} \tag{4-87}$$

for some $\theta_5, \theta_6 \in (0,1)$. Note that $\mathrm{str}^1(P)$ is away from 0 as $p_1 \to 4/d$, and so θ_5, θ_6 are uniformly bounded from below. Thus by the same argument as for (4-67),

$$\|\gamma\|_{\widetilde{\mathcal{Y}}(I)} \le C(A,B)(\varepsilon_0^{\theta_5} + \varepsilon_0^{\theta_6}) \ll \delta. \tag{4-88}$$

Hence under the assumption (4-78) we have obtained

$$\|\gamma\|_{[W]_0(I)\cap[R]_0(I)\cap[\widetilde{N}]_2(I)\cap[P]_2(I)} \lesssim C(A,B)\sum_{k=3}^{6} \varepsilon_0^{\theta_k} \ll \delta. \tag{4-89}$$

Finally by Strichartz, (4-76) and (4-78), we have

$$\begin{aligned}\|u\|_{\mathcal{Y}(I_j)} &\lesssim \|\vec{u}(t_j)\|_{L^2_x} + \|eq(u) + f'(u)\|_{\mathcal{Y}^*(I_j)} \\ &\lesssim A + \varepsilon_0 + \|u\|^{p_1}_{[R]_0(I_j)}\|u\|_{[R]_2(I_j)} + \|u\|^{p_2}_{[M^\sharp]_0(I_j)}\|u\|_{[W]_2(I_j)} \\ &\lesssim A + \varepsilon_0 + \delta^{p_1}\|u\|_{\mathcal{Y}(I_j)}.\end{aligned} \tag{4-90}$$

Hence we obtain

$$\|u\|_{\mathcal{Y}(I_j)} \lesssim A + \varepsilon_0, \tag{4-91}$$

and so

$$\|u\|_{\mathcal{Y}(I)} \lesssim n(A+\varepsilon_0) \le C(A,B), \tag{4-92}$$

which is extended to the full Strichartz norms by Lemma 4.4.

It remains to justify (4-78). By Lemma 4.3(2), we have

$$\|\gamma\|_{[Q]_{2p_1}\cap[\widehat{M}]_2\cap[\widetilde{M}]_{2p_2}} \lesssim \sum_{k=7,8} \|\gamma\|^{1-\theta_k}_{[H]_2\cap[K]_2\cap[W]_2}\|\gamma\|^{\theta_k}_{[P]_2\cap[\widetilde{N}]_2}, \tag{4-93}$$

for some $\theta_7, \theta_8 \in (0,1)$. If $p_1 = 4/d$, then we need to add $[K]_0$ to the last factor.

In either case, by (4-91), (4-76), (4-89), and (4-71), we obtain

$$\|\gamma\|_{([Q]_{2p_1}\cap[\widehat{M}]_2\cap[\widetilde{M}]_{2p_2}\cap[R]_0\cap[M^\sharp]_0)(I_j)} \lesssim C(A,B)\varepsilon_0^{\theta}, \tag{4-94}$$

for some $\theta \in (0,1)$. By choosing $\varepsilon_0(A,B)$ sufficiently small, the last bound can be made much smaller than δ. Then the assumption (4-78) is justified by continuity in t and induction in j. Thus we have obtained the desired estimates. □

5. Profile decomposition

In this section, following Bahouri, Gérard, Kenig, and Merle, we investigate behavior of general sequences of solutions, by asymptotic expansion into a series of transformation sequences of fixed space-time functions, called profiles. This is the fundamental part for the construction of *a critical element* in the next section.

Linear profile decomposition. Here we give the Klein–Gordon version of Bahouri and Gérard's profile decomposition for the massless free wave equation. The only essential difference is that the massive equation does not commute with the scaling transforms, but the proof goes almost the same.

For simple presentation, we introduce some notation. For any triple $(t_\heartsuit^\diamondsuit, x_\heartsuit^\diamondsuit, h_\heartsuit^\diamondsuit) \in \mathbb{R}^{1+d} \times (0,\infty)$ with arbitrary suffix $\heartsuit$ and $\diamondsuit$, let $\tau_\heartsuit^\diamondsuit$, $T_\heartsuit^\diamondsuit$ and $\langle\nabla\rangle_\heartsuit^\diamondsuit$ respectively denote the scaled time shift, the unitary and the self-adjoint operators in $L^2(\mathbb{R}^d)$, defined by

$$\tau_\heartsuit^\diamondsuit = -\frac{t_\heartsuit^\diamondsuit}{h_\heartsuit^\diamondsuit}, \quad T_\heartsuit^\diamondsuit \varphi(x) = (h_\heartsuit^\diamondsuit)^{-d/2}\varphi\left(\frac{x - x_\heartsuit^\diamondsuit}{h_\heartsuit^\diamondsuit}\right), \quad \langle\nabla\rangle_\heartsuit^\diamondsuit = \sqrt{-\Delta + (h_\heartsuit^\diamondsuit)^2}. \tag{5-1}$$

We denote by $\mathcal{MC}$ the set of Fourier multipliers on $\mathbb{R}^d$:

$$\mathcal{MC} = \left\{\mathcal{F}^{-1}\tilde{\mu}\mathcal{F} \mid \tilde{\mu} \in C(\mathbb{R}^d) \text{ and } \tilde{\mu}(x) \text{ has a finite limit as } |x| \to \infty\right\}. \tag{5-2}$$

(Practically we need only 1 and $|\nabla|\langle\nabla\rangle^{-1}$ in $\mathcal{MC}$). Also recall the correspondence $u \leftrightarrow \vec{u}$ defined on page 427.

Lemma 5.1 (Linear profile decomposition). *Let $\vec{v}_n = e^{i\langle\nabla\rangle t}\vec{v}_n(0)$ be a sequence of free Klein–Gordon solutions with bounded L^2_x norm. Then, possibly after replacing it with some subsequence, there exist $K \in \{0, 1, 2\ldots, \infty\}$ and, for each integer $j \in [0, K)$, $\varphi^j \in L^2(\mathbb{R}^d)$ and $\{(t_n^j, x_n^j, h_n^j)\}_{n\in\mathbb{N}} \subset \mathbb{R}\times\mathbb{R}^d \times (0, 1]$ satisfying the following. Define $\vec{v}_n^j$ and $\vec{w}_n^k$ for each $j < k \le K$ by*

$$\vec{v}_n^j = e^{i\langle\nabla\rangle(t-t_n^j)}T_n^j\varphi^j, \quad \vec{v}_n = \sum_{j=0}^{k-1}\vec{v}_n^j + \vec{w}_n^k. \tag{5-3}$$

Then

$$\lim_{k\to K}\ \overline{\lim_{n\to\infty}}\ \|\vec{w}_n^k\|_{L_t^\infty(\mathbb{R}; B^{-d/2}_{\infty,\infty}(\mathbb{R}^d))} = 0, \tag{5-4}$$

and for any Fourier multiplier $\mu \in \mathcal{MC}$, any $l < j < k \le K$ and any $t \in \mathbb{R}$,

$$\lim_{n\to\infty} |\log(h_n^l/h_n^j)| + \frac{|t_n^l - t_n^j| + |x_n^l - x_n^j|}{h_n^l} = \infty, \tag{5-5}$$

$$\lim_{n\to\infty}\langle\mu\vec{v}_n^l(t) \mid \mu\vec{v}_n^j(t)\rangle_{L_x^2} = 0 = \lim_{n\to\infty}\langle\mu\vec{v}_n^j(t) \mid \mu\vec{w}_n^k(t)\rangle_{L_x^2}. \tag{5-6}$$

Moreover, each sequence $\{h_n^j\}_{n\in\mathbb{N}}$ either goes to 0 or is identically 1 for all n.

We call such a sequence $\{\vec{v}_n^j\}_{n\in\mathbb{N}}$ *a free concentrating wave* for each j, and $\vec{w}_n^k$ *the remainder*. We say that $\{(t_n^j, x_n^j, h_n^j)\}_n$ and $\{(t_n^k, x_n^k, h_n^k)\}$ are *orthogonal* when (5-5) holds. Note that (5-6) implies

$$\lim_{n\to\infty}\left[\|\vec{v}_n(t)\|^2_{L_x^2} - \sum_{j<k}\|\vec{v}_n^j(t)\|^2_{L_x^2} - \|\vec{w}_n^k\|^2_{L_x^2}\right] = 0. \tag{5-7}$$

We remark that the case $h_n^j \to \infty$ is excluded by the presence of the mass, or more precisely by the use of inhomogeneous Besov norm for the remainder.

Proof. We introduce a Littlewood–Paley decomposition for the Besov norm. Let $\Lambda_0(x) \in \mathcal{S}(\mathbb{R}^d)$ such that its Fourier transform $\widetilde{\Lambda}_0(\xi) = 1$ for $|\xi| \le 1$ and $\widetilde{\Lambda}_0(\xi) = 0$ for $|\xi| \ge 2$. Then we define $\Lambda_k(x)$ for any $k \in \mathbb{N}$ and $\Lambda_{(0)}(x)$ by the Fourier transforms

$$\widetilde{\Lambda}_k(\xi) = \widetilde{\Lambda}_0(2^{-k}\xi) - \widetilde{\Lambda}_0(2^{-k+1}\xi), \quad \widetilde{\Lambda}_{(0)} = \widetilde{\Lambda}_0(\xi) - \widetilde{\Lambda}_0(2\xi). \tag{5-8}$$

Let

$$\nu := \overline{\lim_{n\to\infty}}\ \|\vec{v}_n\|_{L_t^\infty B^{-d/2}_{\infty,\infty}} \sim \overline{\lim_{n\to\infty}}\ \sup_{t\in\mathbb{R},\ x\in\mathbb{R}^d,\ k\ge 0} 2^{-kd/2}|\Lambda_k * \vec{v}_n(t, x)|. \tag{5-9}$$

If $\nu = 0$, we are done with $K = 0$. Otherwise, there exists a sequence (t_n, x_n, k_n) such that for large n

$$2^{-k_n d/2} |\Lambda_{k_n} * \vec{v}_n(t_n, x_n)| \geq \nu/2. \tag{5-10}$$

Now we define h_n and ψ_n by

$$h_n = 2^{-k_n}, \quad \vec{v}_n(t_n, x) = T_n \psi_n. \tag{5-11}$$

Since ψ_n is bounded in L^2_x, it converges weakly to some ψ in L^2_x, up to an extraction of a subsequence. Moreover,

$$2^{-k_n d/2} |\Lambda_{k_n} * \vec{v}_n(t_n, x_n)| = \begin{cases} |\Lambda_0 * \psi_n(0)| & (k_n = 0), \\ |\Lambda_{(0)} * \psi_n(0)| & (k_n \geq 1), \end{cases} \tag{5-12}$$

and hence by the weak convergence and by Schwarz

$$\|\psi\|_{L^2_x} \gtrsim |\langle \Lambda_0 \mid \psi \rangle| + |\langle \Lambda_{(0)} \mid \psi \rangle| \geq \nu/2. \tag{5-13}$$

If $h_n \to 0$, then we put $(t_n^0, x_n^0, h_n^0) = (t_n, x_n, h_n)$ and $\varphi^0 = \psi$. Otherwise, we may assume, by extracting a subsequence, that h_n converges to some $h_\infty > 0$, and we put

$$(t_n^0, x_n^0, h_n^0) = (t_n, x_n, 1), \quad \varphi^0 = h_\infty^{-d/2} \psi(x/h_\infty). \tag{5-14}$$

Then we have $T_n \psi - T_n^0 \varphi^0 \to 0$ strongly in L^2_x. Now we define $\vec{v}_n^0$ and $\vec{w}_n^1$ by

$$\vec{v}_n^0 = e^{i\langle \nabla \rangle (t - t_n^0)} T_n^0 \varphi^0, \quad \vec{w}_n^1 = \vec{v}_n - \vec{v}_n^0. \tag{5-15}$$

Then $(T_n^0)^{-1} \vec{w}_n^1(t_n^0) = (T_n^0)^{-1} T_n \psi_n - \varphi^0 \to 0$ weakly in L^2, and $\mu T_n^0 = T_n^0 \mu_n^0$, where μ_n^0 denotes the Fourier multiplier whose symbol is the rescaling of μ's, that is $\tilde{\mu}(\xi/h_n^0)$. By the definition of $\mathcal{MC}$, the symbol of μ_n^0 converges, including the case $h_n^0 \to 0$, so μ_n^0 converges strongly in $L^2(\mathbb{R}^d)$ to some μ_∞^0. Hence

$$\langle \mu \vec{v}_n^0(t_n^0) \mid \mu \vec{w}_n^1(t_n^0) \rangle_{L^2_x} = \langle \mu_n^0 \varphi^0 \mid \mu_n^0 (T_n^0)^{-1} \vec{w}_n^1(t_n^0) \rangle_{L^2_x} \to 0. \tag{5-16}$$

The left-hand side is preserved in t, hence the above holds at any t. This is the decomposition for $k = 1$.

Next we apply the same procedure to the sequence $\vec{w}_n^1$ in place of $\vec{v}_n$. Then either the Besov norm goes to 0 and $K = 1$, or otherwise we find the next concentrating wave $\vec{v}_n^1$ and the remainder $\vec{w}_n^2$, such that for some (t_n^1, x_n^1, h_n^1) and $\varphi^1 \in L^2(\mathbb{R}^d)$,

$$\vec{w}_n^1 = \vec{v}_n^1 + \vec{w}_n^2, \quad \vec{v}_n^1 = e^{i\langle \nabla \rangle (t - t_n^1)} T_n^1 \varphi^1, \quad \langle \mu \vec{v}_n^1(t) \mid \mu \vec{w}_n^2(t) \rangle_{L^2_x} \to 0, \tag{5-17}$$

$(T_n^1)^{-1} \vec{w}_n^2(t_n^1) \to 0$ weakly in L^2_x as $n \to \infty$, and

$$\varlimsup_{n \to \infty} \|\vec{w}_n^1\|_{L_t^\infty B^{-d/2}_{\infty,\infty}} \lesssim \|\varphi^1\|_{L^2}. \tag{5-18}$$

Iterating the procedure, we obtain the desired decomposition. L^2 orthogonality implies $\|\varphi^k\|_{L^2_x} \to 0$ as $k \to \infty$, and then (5-18) (for general k) gives the decay of the remainder in the Besov norm.

It remains to prove the orthogonality (5-5) as well as (5-6). First we have

$$\langle \mu \vec{v}_n^l(0) \mid \mu \vec{v}_n^j(0) \rangle = \langle e^{-i\langle \nabla \rangle t_n^l} T_n^l \mu_n^l \varphi^l \mid e^{-i\langle \nabla \rangle t_n^j} T_n^j \mu_n^j \varphi^j \rangle = \langle S_n^{j,l} \mu_n^l \varphi^l \mid \mu_n^j \varphi^j \rangle, \tag{5-19}$$

where $\tilde{\mu}_n^l = \tilde{\mu}(\xi/h_n^l)$ as before, and $S_n^{j,l}$ is defined by

$$S_n^{j,l} := (T_n^j)^{-1} e^{i\langle\nabla\rangle(t_n^j - t_n^l)} T_n^l = e^{-i\langle\nabla\rangle_n^j t_n^{j,l}} (T_n^j)^{-1} T_n^l = e^{-i\langle\nabla\rangle_n^j t_n^{j,l}} T_n^{j,l}, \tag{5-20}$$

with the sequence

$$(t_n^{j,l}, x_n^{j,l}, h_n^{j,l}) := (t_n^l - t_n^j, x_n^l - x_n^j, h_n^l)/h_n^j. \tag{5-21}$$

Using the last formula in (5-20), (5-5), and the uniform time decay of $e^{i\langle\nabla\rangle_n^j t} : \mathcal{S} \to \mathcal{S}'$, it is easy to see that $S_n^{j,l} \to 0$ weakly on L_x^2 as $n \to \infty$ for all $j < l$. Since $\tilde{\mu}_n^l = \tilde{\mu}(\xi/h_n^l)$ and $\tilde{\mu}_n^j$ are convergent, (5-19) also tends to 0. Then we have also

$$\langle \mu \vec{v}_n^j(t) \mid \mu \vec{w}_n^k(t)\rangle_{L_x^2} = \Big\langle \mu \vec{v}_n^j(t) \mid \mu \vec{w}_n^{j+1}(t) - \sum_{m=j+1}^{k-1} \mu \vec{v}_n^m(t)\Big\rangle_{L_x^2} \to 0; \tag{5-22}$$

thus we obtain (5-6). Now suppose that (5-5) fails. Then there exists a minimal (l, j) breaking (5-5), with respect to the natural order

$$(l_1, j_1) \le (l_2, j_2) \iff l_1 \le l_2 \text{ and } j_1 \le j_2. \tag{5-23}$$

By extracting a subsequence, we may assume that $h_n^l \to h_\infty^l$, $\log(h_n^l/h_n^j)$, $(t_n^l - t_n^j)/h_n^l$ and $(x_n^l - x_n^j)/h_n^l$ all converge. Now we inspect

$$(T_n^l)^{-1} \vec{w}_n^{l+1}(t_n^l) = \sum_{m=l+1}^{j} S_n^{l,m} \varphi^m + S_n^{l,j} (T_n^j)^{-1} \vec{w}_n^{j+1}(t_n^j). \tag{5-24}$$

where $S_n^{l,j}$ converges strongly to a unitary operator, due to the convergence of $(t_n^{l,j}, x_n^{l,j}, h_n^{l,j})$ and h_n^l. Since $S_n^{l,m} \to 0$ for $m < j$ and $(T_n^j)^{-1} \vec{w}_n^{j+1}(t_n^j) \to 0$ weakly in L_x^2, we deduce from the weak limit of (5-24) that $\varphi^k = 0$, a contradiction. This proves the orthogonality (5-5). □

Those free concentrating waves with scaling going to 0 are vanishing in any Besov space with less regularity. Hence in the subcritical case, we may freeze the scaling to 1 by regarding them as a part of remainder. Hence:

Corollary 5.2. *Let $\vec{v}_n$ be a sequence of free Klein–Gordon solutions with bounded L_x^2 norm. Then, after replacing it with some subsequence, there exist $K \in \{0, 1, 2 \dots, \infty\}$ and data $\varphi^j \in L^2(\mathbb{R}^d)$ and $\{(t_n^j, x_n^j)\}_{n\in\mathbb{N}} \subset \mathbb{R} \times \mathbb{R}^d$, for each integer $j \in [0, K)$, satisfying the following. Define $\vec{v}_n^j$ and $\vec{w}_n^k$ for each $j < k \le K$ by*

$$\vec{v}_n^j = e^{i\langle\nabla\rangle(t - t_n^j)} \varphi^j(x - x_n^j), \quad \vec{v}_n = \sum_{j=0}^{k-1} \vec{v}_n^j + \vec{w}_n^k. \tag{5-25}$$

Then, for any $s < -d/2$, we have

$$\lim_{k\to K} \varlimsup_{n\to\infty} \|\vec{w}_n^k\|_{L^\infty(\mathbb{R}; B^s_{\infty,1}(\mathbb{R}^d))} = 0, \tag{5-26}$$

and for any $\mu \in \mathcal{MC}$, any $l < j < k \le K$ and any $t \in \mathbb{R}$,

$$\lim_{n\to\infty} \langle \mu \vec{v}_n^l \mid \mu \vec{v}_n^j \rangle_{L_x^2}^2 = 0 = \lim_{n\to\infty} \langle \mu \vec{v}_n^j \mid \mu \vec{w}_n^k \rangle_{L_x^2}, \tag{5-27}$$

$$\lim_{n\to\infty} |t_n^j - t_n^k| + |x_n^j - x_n^k| = \infty. \tag{5-28}$$

Orthogonality holds also for the nonlinear energy, which implies that the decomposition is closed in $\widetilde{\mathcal{K}}^+$. Recall the vector notation for the energy (page 427). We will use the following estimates for $1 < p < \infty$:

$$\begin{aligned} \|[|\nabla| - \langle\nabla\rangle_n]\varphi\|_{L^p_x} &\lesssim h_n \|\langle\nabla/h_n\rangle^{-1}\varphi\|_{L^p_x}, \\ \|[|\nabla|^{-1} - \langle\nabla\rangle_n^{-1}]\varphi\|_{L^p_x} &\lesssim \|\langle\nabla/h_n\rangle^{-2}|\nabla|^{-1}\varphi\|_{L^p_x}; \end{aligned} \tag{5-29}$$

they hold uniformly for $0 < h_n \le 1$, by Mihlin's theorem on Fourier multipliers.

Lemma 5.3. *Assume that f satisfies* (1-36). *Let $\vec{v}_n$ be a sequence of free Klein–Gordon solutions satisfying $\vec{v}_n(0) \in \widetilde{\mathcal{K}}^+$ and $\overline{\lim}_{n\to\infty} \widetilde{E}(\vec{v}_n(0)) < m$. Let $\vec{v}_n = \sum_{j<k} \vec{v}_n^j + \vec{w}_n^k$ be the linear profile decomposition given by Lemma 5.1. Except for the H^1 critical case* (1-28), *it may be given by Corollary 5.2 too. Then we have $\vec{v}_n^j(0) \in \widetilde{\mathcal{K}}^+$ for large n and all $j < K$, and*

$$\lim_{k\to K} \overline{\lim_{n\to\infty}} \left| \widetilde{E}(\vec{v}_n(0)) - \sum_{j<k} \widetilde{E}(\vec{v}_n^j(0)) - \widetilde{E}(\vec{w}_n^k(0)) \right| = 0. \tag{5-30}$$

Moreover we have for all $j < K$

$$0 \le \underline{\lim}_{n\to\infty} \widetilde{E}(\vec{v}_n^j(0)) \le \overline{\lim_{n\to\infty}} \widetilde{E}(\vec{v}_n^j(0)) \le \overline{\lim_{n\to\infty}} \widetilde{E}(\vec{v}_n(0)), \tag{5-31}$$

where the last inequality becomes an equality only if $K = 1$ and $\vec{w}_n^1 \to 0$ in $L_t^\infty L_x^2$.

Proof. First we see that in the exponential case (1-29), all the profiles and remainders are in the subcritical regime. Since $\vec{v}_n(0) \in \widetilde{\mathcal{K}}^+$, Lemma 2.11 implies

$$\|\nabla\langle\nabla\rangle^{-1} \operatorname{Re} \vec{v}_n(0)\|_{L_x^2}^2 + \|\operatorname{Im} \vec{v}_n(0)\|_{L_x^2}^2 < 2m \le 4\pi/\kappa_0. \tag{5-32}$$

For any $(\theta_0, \dots, \theta_k) \in \mathbb{C}^{1+k}$ satisfying $\|\theta\|_{L^\infty} = \max_j |\theta_j| \le 1$, let

$$v_n^\theta = \sum_{j<k} \theta_j v_n^j + \theta_k w_n^k. \tag{5-33}$$

Choosing $\mu = |\nabla|\langle\nabla\rangle^{-1} \in \mathcal{MC}$ in (5-27), we get

$$\overline{\lim_{n\to\infty}} \sup_{t\in\mathbb{R}} \|\nabla v_n^\theta\|_{L_x^2}^2 \le \overline{\lim_{n\to\infty}} \|\nabla\langle\nabla\rangle^{-1}\vec{v}_n\|_{L_x^2}^2 =: M < 4\pi/\kappa_0. \tag{5-34}$$

Hence there exist $\kappa > \kappa_0$ and $q \in (1, 2)$ such that $q\kappa M < 4\pi$.

Now we start proving (5-30) in all the cases. Since the linear version of (5-30) is given by Lemma 5.1, it suffices to show orthogonality in F, i.e.

$$\lim_{k\to K} \overline{\lim_{n\to\infty}} \left| F(v_n(0)) - \sum_{j<k} F(v_n^j(0)) - F(w_n^k(0)) \right| = 0. \tag{5-35}$$

For this we may neglect w_n^k, because by the decay in $B^{1-d/2}_{\infty,\infty}$ and interpolation with the H^1 bound we have

$$\lim_{k\to K} \overline{\lim_{n\to\infty}} \|w_n^k(0)\|_{L_x^p} = 0 \quad (2 < p \le 2^\star). \tag{5-36}$$

In the exponential case, we deal with w_n^k as follows. Let $v_n^{<k+\theta} = v_n - (1-\theta)w_n^k$ for $0 \le \theta \le 1$. Using

the Hölder and Trudinger–Moser inequalities, we get

$$\begin{aligned}|F(v_n)-F(v_n^{<k})| &\le \int_0^1\int |f'(v_n^{<k+\theta})w_n^k|\,dx\,d\theta \le \int_0^1 d\theta\,\|e^{q\kappa|v_n^{<k+\theta}|^2}-1\|_{L^1_x}^{1/q}\|w_n^k\|_{L^{q'}_x}\\ &\le \int_0^1 d\theta\left[\frac{\|v_n^{<k+\theta}\|_{L^2_x}^2}{4\pi-q\kappa M}\right]^{1/q}\|w_n^k\|_{L^{q'}_x}.\end{aligned} \tag{5-37}$$

In the subcritical and exponential cases, it suffices to have the decay in $B^s_{\infty,1}$ for all $s<1-d/2$, which is given by Corollary 5.2. Thus in any case we are allowed to replace $v_n(0)$ by $v_n^{<k}(0)$ in (5-35).

Next we may discard those j for which $\tau_n^j=-t_n^j/h_n^j\to\pm\infty$, since for any $p\in(2,2^\star]$ satisfying $1/p=1/2-s/d$ with $s\in(0,1]$, we have

$$\|v_n^j(0)\|_{L^p_x}\lesssim\|e^{-i\langle\nabla\rangle_n^j\tau_n^j}|\nabla|^{-s}\varphi^j\|_{L^p_x}\to 0\quad(n\to\infty), \tag{5-38}$$

by the decay of $e^{i\langle\nabla\rangle_n^j t}$ in $\mathcal{S}\to L^p$ as $|t|\to\infty$, which is uniform in n, and the Sobolev embedding $\dot H^s_x\subset L^p_x$.

So extracting a subsequence, we may assume that τ_n^j has a finite limit τ_∞^j for all j. Let

$$\psi^j:=\operatorname{Re}e^{-i\langle\nabla\rangle_\infty^j\tau_\infty^j}\varphi^j\in L^2_x(\mathbb{R}^d). \tag{5-39}$$

Then $v_n^j(0)-\langle\nabla\rangle^{-1}T_n^j\psi^j\to 0$ strongly in H^1_x, thus (5-35) has been reduced to

$$\left|F\Big(\sum_{j<k}\langle\nabla\rangle^{-1}T_n^j\psi^j\Big)-\sum_{j<k}F(\langle\nabla\rangle^{-1}T_n^j\psi^j)\right|\to 0. \tag{5-40}$$

In the subcritical and exponential cases, if $h_n^j\to 0$ then $\langle\nabla\rangle^{-1}T_n^j\psi^j\to 0$ strongly in L^p_x for $2\le p<2^\star$, so it can be neglected. Hence we may assume that $h_n^j\equiv 1$. Then each $T_n^j\langle\nabla\rangle^{-1}\psi^j$ is getting away from the others as $n\to\infty$, and (5-40) follows.

In the critical case, if $h_n^j\to 0$ then we have by (5-29),

$$\|\langle\nabla\rangle^{-1}T_n^j\psi^j-h_n^jT_n^j|\nabla|^{-1}\psi^j\|_{L^{2^\star}_x}\lesssim\|\langle\nabla/h_n^j\rangle^{-2}|\nabla|^{-1}\psi^j\|_{L^{2^\star}_x}\to 0. \tag{5-41}$$

Hence we may replace $\langle\nabla\rangle^{-1}T_n^j\psi^j$ in (5-40) by $h_n^jT_n^j\hat\psi^j$ for some $\hat\psi^j\in L^{2^\star}$, including the case $h_n^j\equiv 1$. Then we may further replace each $\hat\psi^j$ by

$$\check\psi_n^j(x):=\hat\psi^j(x)\times\begin{cases}0 & \text{if there is } l<j \text{ s.t. } h_n^l<h_n^j \text{ and } (x-x_n^{j,l})/h_n^{j,l}\in\operatorname{supp}\hat\psi^l,\\ 1 & \text{otherwise,}\end{cases} \tag{5-42}$$

where $(x_n^{j,l},h_n^{j,l})$ is defined in (5-21), because (5-5) after the above reduction implies either $h_n^{j,l}\to 0$ or $|x_n^{j,l}|\to\infty$, and so $\check\psi^j\to\hat\psi^j$ at almost every $x\in\mathbb{R}^d$ as $n\to\infty$, and strongly in $L^{2^\star}_x$ by the dominated convergence theorem. Now the decomposition is trivial

$$F\Big(\sum_{j<k}h_n^jT_n^j\check\psi_n^j\Big)=\sum_{j<k}F(h_n^jT_n^j\check\psi_n^j), \tag{5-43}$$

by the support property of $\check\psi_n^j$. Thus we have obtained (5-35) and (5-30).

By exactly the same argument, we obtain also

$$\lim_{k\to K}\varlimsup_{n\to\infty}\Big|\widetilde{K}_{\alpha,\beta}(\vec{v}_n(0))-\sum_{j<k}\widetilde{K}_{\alpha,\beta}(\vec{v}_n^{\,j}(0))-\widetilde{K}_{\alpha,\beta}(\vec{w}_n^{\,k}(0))\Big|=0. \tag{5-44}$$

The remaining conclusions follow from the next lemma. □

Lemma 5.4 (Decomposition in $\widetilde{\mathcal{K}}^+$). *Assume f satisfies* (1-36). *Let $k\in\mathbb{N}$ and $\varphi_0,\dots,\varphi_k\in H^1(\mathbb{R}^d)$. Assume that*

$$\begin{aligned}&\widetilde{E}\Big(\sum_{j=0}^{k}\varphi_j\Big)\le m-\delta, &&\widetilde{K}_{\alpha,\beta}\Big(\sum_{j=0}^{k}\varphi_j\Big)\ge-\varepsilon,\\ &\widetilde{E}\Big(\sum_{j=0}^{k}\varphi_j\Big)\ge\sum_{j=0}^{k}\widetilde{E}(\varphi_j)-\varepsilon, &&\widetilde{K}_{\alpha,\beta}\Big(\sum_{j=0}^{k}\varphi_j\Big)\le\sum_{j=0}^{k}\widetilde{K}_{\alpha,\beta}(\varphi_j)+\varepsilon,\end{aligned} \tag{5-45}$$

for some (α,β) in (1-16) *and some $\delta,\varepsilon>0$ satisfying $\varepsilon(1+2/\bar{\mu})<\delta$. Then $\tilde{\varphi}_j\in\widetilde{\mathcal{K}}^+$ for all $j=0,\dots,k$, i.e. $0\le\widetilde{E}(\varphi_j)<m$ and $\widetilde{K}_{\alpha,\beta}(\varphi_j)\ge0$ for all (α,β) in* (1-16).

Proof. Let $\psi_j=\operatorname{Re}\langle\nabla\rangle^{-1}\varphi_j$ and suppose that $\widetilde{K}(\varphi_l)<0$ for some l. Then $K(\psi_l)\le\widetilde{K}(\varphi_l)<0$ and so $H(\psi_l)\ge m$. Since H is non-negative,

$$\begin{aligned}m\le\sum_{j=0}^{k}H(\psi_j)&\le\sum_{j=0}^{k}[H(\psi_j)+H^Q(\operatorname{Im}\langle\nabla\rangle^{-1}\varphi_j)]=\sum_{j=0}^{k}[\widetilde{E}(\varphi_j)-\widetilde{K}(\varphi_j)/\bar{\mu}]\\ &\le\widetilde{E}\Big(\sum_{j=0}^{k}\varphi_j\Big)-\widetilde{K}\Big(\sum_{j=0}^{k}\varphi_j\Big)/\bar{\mu}+\varepsilon(1+1/\bar{\mu})<m,\end{aligned} \tag{5-46}$$

where H^Q denotes the quadratic part of H. Hence $K(\psi_j)\ge0$ for all j, and so

$$\widetilde{E}(\varphi_j)\ge J(\psi_j)=H(\psi_j)+K(\psi_j)/\bar{\mu}\ge0.$$ □

Nonlinear profile decomposition. The next step is to construct a similar decomposition for the nonlinear solutions with the same initial data.

First we construct a nonlinear profile corresponding to a free concentrating wave. Let $\vec{v}_n$ be a free concentrating wave for a sequence $(t_n,x_n,h_n)\in\mathbb{R}\times\mathbb{R}^d\times(0,1]$,

$$(i\partial_t+\langle\nabla\rangle)\vec{v}_n=0,\quad \vec{v}_n(t_n)=T_n\psi,\quad \psi(x)\in L^2, \tag{5-47}$$

satisfying $\vec{v}_n(0)\in\widetilde{\mathcal{K}}^+$. Here we use Lemma 5.1 only in the H^1 critical case, and Corollary 5.2 in the subcritical and exponential cases. Hence $h_n\to0$ can happen only in the critical case, otherwise $h_n\equiv1$. Let u_n be the nonlinear solution with the same initial data

$$(i\partial_t+\langle\nabla\rangle)\vec{u}_n=f'(u_n),\quad \vec{u}_n(0)=\vec{v}_n(0)\in\widetilde{\mathcal{K}}^+, \tag{5-48}$$

which may be local in time. Next we define $\vec{V}_n$ and $\vec{U}_n$ by undoing the transforms

$$\vec{v}_n=T_n\vec{V}_n((t-t_n)/h_n),\quad \vec{u}_n=T_n\vec{U}_n((t-t_n)/h_n). \tag{5-49}$$

Then they satisfy the rescaled equations

$$\vec{V}_n = e^{it\langle\nabla\rangle_n}\psi, \quad \vec{U}_n = \vec{V}_n - i\int_{\tau_n}^t e^{i(t-s)\langle\nabla\rangle_n} f'(\mathrm{Re}\langle\nabla\rangle_n^{-1}\vec{U}_n)\,ds, \tag{5-50}$$

where $\tau_n = -t_n/h_n$. Extracting a subsequence, we may assume convergence:

$$h_n \to h_\infty \in [0,1], \quad \tau_n \to \tau_\infty \in [-\infty,\infty]. \tag{5-51}$$

Then the limit equations are naturally given by

$$\vec{V}_\infty = e^{it\langle\nabla\rangle_\infty}\psi, \quad \vec{U}_\infty = \vec{V}_\infty - i\int_{\tau_\infty}^t e^{i(t-s)\langle\nabla\rangle_\infty} f'(\widehat{U}_\infty)\,ds, \tag{5-52}$$

where $\widehat{U}_\infty$ is defined by

$$\widehat{U}_\infty := \mathrm{Re}\langle\nabla\rangle_\infty^{-1}\vec{U}_\infty = \begin{cases}\mathrm{Re}\langle\nabla\rangle^{-1}\vec{U}_\infty & (h_\infty = 1),\\ \mathrm{Re}\,|\nabla|^{-1}\vec{U}_\infty & (h_\infty = 0).\end{cases} \tag{5-53}$$

The unique existence of a local solution $\vec{U}_\infty$ around $t = \tau_\infty$ is known in all cases, including $h_\infty = 0$ and $\tau_\infty = \pm\infty$ (the latter corresponding to the existence of the wave operators), by using the standard iteration with the Strichartz estimate. In the exponential case, it requires that $\vec{U}_\infty$ is in the subcritical regime in the Trudinger–Moser inequality. It is guaranteed by Lemma 5.3, because $\vec{V}_\infty(t) \in \widetilde{\mathcal{K}}^+$ for t close to τ_∞, and so $\vec{U}_\infty(t) \in \widetilde{\mathcal{K}}^+$ for all t in its existence interval.

$\vec{U}_\infty$ on the maximal existence interval is called the *nonlinear profile* associated with the free concentrating wave $\vec{v}_n$. The *nonlinear concentrating wave* $\vec{u}_{(n)}$ associated with $\vec{v}_n$ is defined by

$$\vec{u}_{(n)} = T_n\vec{U}_\infty((t-t_n)/h_n). \tag{5-54}$$

If $h_\infty = 1$ then $u_{(n)}$ solves NLKG. If $h_\infty = 0$ then it solves

$$(\partial_t^2 - \Delta + 1)u_{(n)} = (i\partial_t + \langle\nabla\rangle)\vec{u}_{(n)} = (\langle\nabla\rangle - |\nabla|)\vec{u}_{(n)} + f'(|\nabla|^{-1}\langle\nabla\rangle u_{(n)}). \tag{5-55}$$

The existence time of $u_{(n)}$ may be finite and even go to 0, but at least we have

$$\begin{aligned}\|\vec{u}_n(0) - \vec{u}_{(n)}(0)\|_{L^2_x} &= \|\vec{V}_n(\tau_n) - \vec{U}_\infty(\tau_n)\|_{L^2_x}\\ &\le \|\vec{V}_n(\tau_n) - \vec{V}_\infty(\tau_n)\|_{L^2_x} + \|\vec{V}_\infty(\tau_n) - \vec{U}_\infty(\tau_n)\|_{L^2_x} \to 0.\end{aligned} \tag{5-56}$$

Let u_n be a sequence of (local) solutions of NLKG in $\mathcal{K}^+$ around $t = 0$, and let v_n be the sequence of the free solutions with the same initial data. We consider the linear profile decomposition given by Lemma 5.1 or 5.2:

$$\vec{v}_n = \sum_{j=0}^{k-1} \vec{v}_n^j + \vec{w}_n^k, \quad \vec{v}_n^j = e^{i\langle\nabla\rangle(t-t_n^j)}T_n^j\varphi^j. \tag{5-57}$$

With each free concentrating wave $\{\vec{v}_n^j\}_{n\in\mathbb{N}}$, we associate the nonlinear concentrating wave $\{\vec{u}_{(n)}^j\}_{n\in\mathbb{N}}$. A *nonlinear profile decomposition* of u_n is given by

$$\vec{u}_{(n)}^{<k} := \sum_{j=0}^{k-1} \vec{u}_{(n)}^j. \tag{5-58}$$

We are going to prove that $\vec{u}_{(n)}^{<k}$ is a good approximation for $\vec{u}_n$, provided that each nonlinear profile has finite global Strichartz norm (in Lemma 5.6). Now we define the Strichartz norms for the profile decomposition, using the notation from page 428. Let ST and ST^* be the function spaces on $\mathbb{R}^{1+d}$ defined by

$$ST = [W]_2 \cap [K]_2, \quad ST^* = [W^{*(1)}]_2 + [K^{*(1)}]_2 + L_t^1 L_x^2, \tag{5-59}$$

where the exponents W and K as well as their duals are as defined in (4-24) and (4-9). The Strichartz norm for the nonlinear profile depends on the scaling $h_\infty^\diamond$ for any suffix $\diamond$:

$$ST_\infty^\diamond := \begin{cases} [W]_2 \cap [K]_2 & (h_\infty^\diamond = 1), \\ [W]_2^\bullet & (h_\infty^\diamond = 0). \end{cases} \tag{5-60}$$

In other words, we take the scaling invariant part if $h_n^\diamond \to +0$, which can happen only in the H^1 critical case. The following estimate will be convenient in treating the concentrating case: For any $S \in [0,1] \times [0, \frac{1}{2}] \times [0,1]$ we have

$$\|u_{(n)}\|_{[S]_2(\mathbb{R})} \lesssim (h_n)^{1-\mathrm{reg}^0(S)} \|\widehat{U}_\infty\|_{[S]_2^\bullet(\mathbb{R})}, \tag{5-61}$$

where $\widehat{U}_\infty$ is as defined in (5-53). Indeed, using $\dot{B}^0_{p,2} \subset L^p$ with $p = 1/S_2 \geq 2$ in the lower frequencies, we have

$$\begin{aligned} \|u_{(n)}\|_{[S]_2} &\lesssim \||\nabla|^{-S_3} \langle\nabla\rangle^{S_3} u_{(n)}\|_{[S]_2^\bullet} \\ &\sim (h_n)^{1-\mathrm{reg}^0(S)} \|\operatorname{Re} |\nabla|^{-S_3} \langle\nabla\rangle_n^{S_3-1} \vec{U}_\infty^j\|_{[S]_2^\bullet} \lesssim (h_n)^{1-\mathrm{reg}^0(S)} \|\widehat{U}_\infty^j\|_{[S]_2^\bullet}. \end{aligned} \tag{5-62}$$

Concerning the orthogonality in the Strichartz norms, we have:

Lemma 5.5. *Assume that f satisfies* (1-36). *Suppose that in the nonlinear profile decomposition* (5-58) *we have*

$$\|\widehat{U}_\infty^j\|_{ST_\infty^j(\mathbb{R})} + \|\vec{U}_\infty^j\|_{L_t^\infty L_x^2(\mathbb{R})} < \infty \tag{5-63}$$

for each $j < K$. Then, for any finite interval I, any $j < K$ and any $k \leq K$, we have

$$\varlimsup_{n\to\infty} \|u_{(n)}^j\|_{ST(I)} \lesssim \|\widehat{U}_\infty^j\|_{ST_\infty^j(\mathbb{R})}, \tag{5-64}$$

$$\varlimsup_{n\to\infty} \|u_{(n)}^{<k}\|_{ST(I)}^2 \lesssim \varlimsup_{n\to\infty} \sum_{j<k} \|u_{(n)}^j\|_{ST(I)}^2, \tag{5-65}$$

where the implicit constants do not depend on I, j or k. We also have

$$\lim_{n\to\infty} \Big\| f'(u_{(n)}^{<k}) - \sum_{j<k} f'\big((\langle\nabla\rangle_\infty^j)^{-1} \langle\nabla\rangle u_{(n)}^j\big) \Big\|_{ST^*(I)} = 0. \tag{5-66}$$

Proof. First note that if $h_\infty^j = 1$ then $u_{(n)}^j$ is just a sequence of space-time translations of $\widehat{U}_\infty^j$. In particular, (5-64) is trivial in that case.

Next we prove (5-64) in the case $h_\infty^j = 0$, which is only in the H^1 critical case. For the moment we drop the superscript j. For the $[W]_2$ part, (5-61) gives us

$$\|u_{(n)}\|_{[W]_2(I)} \lesssim \|\widehat{U}_\infty\|_{[W]_2^\bullet(\mathbb{R})} = \|\widehat{U}_\infty\|_{ST_\infty^j(\mathbb{R})}. \tag{5-67}$$

For the $[K]_2$ part, let V be the following interpolation between H and W

$$V := \frac{1}{d+2}H + \frac{d+1}{d+2}W = K + \frac{(-1,0,1)}{2(d+2)}. \tag{5-68}$$

Then using Hölder in t and (5-61) together with $\mathrm{reg}^0(K) = (d+1)/(d+2)$, we get

$$\|u_{(n)}\|_{[K]_2(I)} \lesssim \|u_{(n)}\|_{[V^{\frac{1}{2}}]_2(I)} |I|^{\frac{1}{2(d+2)}} \lesssim (h_n)^{\frac{1}{2(d+2)}} \|\widehat{U}_\infty\|_{[V]_2^\bullet(\mathbb{R})} |I|^{\frac{1}{2(d+2)}} \to 0, \tag{5-69}$$

as $n \to \infty$. Thus we have proved (5-64).

Next we prove (5-65) in the subcritical and exponential cases. Define $\widehat{U}^j_{\infty,R}$, $u^j_{(n),R}$ for $R \gg 1$ and $u^{<k}_{(n),R}$ by

$$\widehat{U}^j_{\infty,R} = \chi_R(t,x)\widehat{U}^j_\infty, \quad u^j_{(n),R} = T^j_n \widehat{U}^j_{\infty,R}(t-t^j_n), \quad u^{<k}_{(n),R} = \sum_{j<k} u^j_{(n),R}, \tag{5-70}$$

where χ_R is the cut-off defined in (1-23). Then we have

$$\|u^{<k}_{(n)} - u^{<k}_{(n),R}\|_{ST(\mathbb{R})} \le \sum_{j<k} \|(1-\chi_R(t,x))\widehat{U}^j_\infty\|_{ST(\mathbb{R})} \to 0, \quad (R \to +0) \tag{5-71}$$

so we may replace $u^{<k}_{(n)}$ by $u^{<k}_{(n),R}$. Let δ^l_m denote the difference operator

$$\delta^l_m \varphi(x) = \varphi(x - 2^{-m}e_l) - \varphi(x), \tag{5-72}$$

where e_l denotes the l-th unit vector in $\mathbb{R}^d$. Each Besov norm in ST is equivalent to

$$\sum_{l=1}^d \Big\| \sum_{j<k} 2^{sm}\delta^l_m u^j_{(n),R} \Big\|_{L^p_t \ell^2_{m\ge 0} L^q_x} + \Big\| \sum_{j<k} u^j_{(n),R} \Big\|_{L^p_t L^q_x}, \tag{5-73}$$

where $(1/p, 1/q, s) = W$ or K. (5-28) implies that each $\operatorname{supp} u^j_{(n),R}$ is away from the others at least by distance 2 for large n, and then $\operatorname{supp} \delta^l_m u^j_{(n),R}$ are also disjoint for $j < k$ at each l, m. Hence the first norm in (5-73) equals

$$\|2^{sm}\delta^l_m u^j_{(n),R}\|_{L^p_t \ell^2_{m\ge 0} L^q_x \ell^2_{j<k}} \le \|2^{sm}\delta^l_m u^j_{(n),R}\|_{\ell^2_{j<k} L^p_t \ell^2_{m\ge 0} L^q_x} \lesssim \|u^j_{(n),R}\|_{\ell^2_{j<k} L^p_t B^s_{q,2}}, \tag{5-74}$$

where the first inequality is by Minkowski. Thus we have obtained (5-65) in the subcritical and exponential cases.

Next we prove (5-65) in the H^1 critical case. For the nonlinear concentrating waves with $h^j_\infty = 1$, the above argument works. For those with $h^j_\infty = 0$, the K component is vanishing by (5-69). Hence it suffices to estimate $[W]_2$ in the case all h^j_n tend to 0 as $j \to \infty$. Using that $W_3 = \frac{1}{2} \in (0,1)$, we have

$$\big\|u^{<k}_{(n)}\big\|_{[W]_2(\mathbb{R})} \lesssim \big\||\nabla|^{-1}\langle\nabla\rangle u^{<k}_{(n)}\big\|_{[W]_2^\bullet(\mathbb{R})} = \big\|\operatorname{Re}|\nabla|^{-1}\vec{u}^{<k}_{(n)}\big\|_{[W]_2^\bullet(\mathbb{R})} \sim \Big\|\sum_{j<k} \check{u}^{j,l}_{n,m}\Big\|_{L^p_t \ell^2_{m\in\mathbb{Z}} L^q_x}, \tag{5-75}$$

where we have put $(1/p, 1/q, s) = W$ and

$$\check{u}^{j,l}_{n,m} := 2^{sm}\delta^l_m h^j_n T^j_n \widehat{U}^j_\infty((t-t^j_n)/h^j_n), \tag{5-76}$$

where δ_m^l is the difference operator defined in (5-72). For $R \gg 1$, let

$$\check{u}_{n,m,R}^{j,l}(t,x) := \begin{cases} \chi_{h_n^j R}(t-t_n^j, x-x_n^j)\check{u}_{n,m}^{j,l}(t,x) & (|m-\log_2 h_n^j| \le R) \\ 0 & (|m-\log_2 h_n^j| > R), \end{cases} \tag{5-77}$$

where χ_* is as in (1-23). Then by the same computation as for (5-61), we have

$$\|\check{u}_{n,m}^{j,l} - \check{u}_{n,m,R}^{j,l}\|_{L_t^p \ell^2_{m\in\mathbb{Z}} L_x^q} \lesssim \|2^{sm}\delta_m^l \widehat{U}_\infty^j\|_{L_t^p \ell_m^2 L_x^q(|t|+|m|+|x|>R)} \to 0, \tag{5-78}$$

as $R \to \infty$ uniformly in n. Hence we may replace $\check{u}_{n,m}^{j,l}$ by $\check{u}_{n,m,R}^{j,l}$ in (5-75). The orthogonality (5-5) implies that $\{\mathrm{supp}_{(t,m,x)}\, \check{u}_{n,m,R}^{j,l}\}_{j<k}$ becomes mutually disjoint for large n. Then arguing as in (5-74), we obtain (5-65).

To prove (5-66) in the subcritical and exponential cases is easier than (5-65), because after the smooth cut-off, we have for large n

$$f'(u_{(n),R}^{<k}) = \sum_{j<k} f'(u_{(n),R}^j). \tag{5-79}$$

Note that the $u_{(n)}^j \in ST$ implies that the full Strichartz norms are finite by Lemma 4.4. The error for $f'(u_{(n)}^{<k})$ coming from the cut-off is small in ST^* by (4-61)–(4-64) if $d \le 4$. When $d \ge 5$, the difference estimates in the proof of Lemma 4.5 are not sufficient because they control only the exotic norm Y. In order to estimate the difference in the admissible dual norm $ST^*(I)$, we introduce the new exponents

$$H_\varepsilon := \Big(\varepsilon^2, \frac{1-\varepsilon}{2}, 0\Big), \quad W_\varepsilon := W - p_2\varepsilon(d,-1,0), \quad M_\varepsilon^\sharp := M^\sharp + \varepsilon(d,-1,0), \tag{5-80}$$

where W and $M^\sharp$ were defined in (4-24) and (4-31), and $\varepsilon \in (0, p_1)$ is fixed small enough to have

$$\begin{aligned} &\mathrm{str}^0(H_\varepsilon), \mathrm{str}^0(M_\varepsilon^\sharp), \mathrm{str}^0(W_\varepsilon) < 0, \quad \mathrm{reg}^0(H_\varepsilon) < 1, \\ &\mathrm{reg}^0(W_\varepsilon) = \mathrm{reg}^0(W) = 1, \quad \mathrm{reg}^0(M_\varepsilon^\sharp) = \mathrm{reg}^0(M^\sharp) \le 1, \\ &W_\varepsilon + p_2 M_\varepsilon^\sharp = W + p_2 M^\sharp = W^{*(1)}. \end{aligned} \tag{5-81}$$

Then we have, for any u and v,

$$\|f_S'(u) - f_S'(v)\|_{L_t^1 L_x^2(I)} \lesssim |I|^{1-\varepsilon^2} \|u-v\|_{[H_\varepsilon]_0(I)} \big(\|u\|_{L_t^\infty L_x^2(I)} + \|v\|_{L_t^\infty L_x^2(I)}\big)^\varepsilon, \tag{5-82}$$

because $|f_S'(u) - f_S'(v)| \lesssim |u-v|(|u|+|v|)^\varepsilon$. For large u, we have if $p_2 \ge 1$,

$$\begin{aligned} &\|f_L'(u) - f_L'(v)\|_{[W^{*(1)}]_2} \\ &\quad\lesssim \|u\|_{[M_\varepsilon^\sharp]_0}^{p_2} \|u-v\|_{[W_\varepsilon]_2} + \|u-v\|_{[M_\varepsilon^\sharp]_0} \big(\|u\|_{[M_\varepsilon^\sharp]_0} + \|v\|_{[M_\varepsilon^\sharp]_0}\big)^{p_2-1} \|v\|_{[W_\varepsilon]_2}, \end{aligned} \tag{5-83}$$

and if $p_2 < 1$,

$$\|f_L'(u) - f_L'(v)\|_{[W_\varepsilon^{*(1)}]_2} \lesssim \|u\|_{[M_\varepsilon^\sharp]_0}^{p_2} \|u-v\|_{[W_\varepsilon]_2} + \|u-v\|_{[M_\varepsilon^\sharp]_0}^{p_2} \|v\|_{[W_\varepsilon]_2}. \tag{5-84}$$

The latter estimate is not Lipschitz in $u-v$, but suffices for our purpose here.[4] Thus we obtain (5-66) in the subcritical and exponential cases.

[4]The situation is different from the long-time iteration in the previous section, where we needed the exotic Strichartz estimate in order to get the Lipschitz estimate for the iteration along the numerous time intervals.

It remains to prove (5-66) in the H^1 critical case, where we need further cut-off to get a disjoint sum. First we see that each $u^j_{(n)}$ in $u^{<k}_{(n)}$ may be replaced with

$$u^j_{\langle n\rangle} := (\langle\nabla\rangle^j_\infty)^{-1}\langle\nabla\rangle u^j_{(n)} = h^j_n T^j_n \widehat{U}^j_\infty((t-t^j_n)/h^j_n). \tag{5-85}$$

For the moment we drop the superscript j. Let $p_2 = 4/(d-2)$ and $h_\infty = 0$. If $d \le 4$, then we have by using (4-62) and (5-29)

$$\begin{aligned}\|f'(u_{(n)}) - f'(u_{\langle n\rangle})\|_{L^1_t L^2_x(\mathbb{R})} &\lesssim \|u_{\langle n\rangle}\|^{p_2}_{[L]_0(\mathbb{R})}\|u_{(n)} - u_{\langle n\rangle}\|_{[L]_0(\mathbb{R})} \\ &\sim \|\widehat{U}_\infty\|^{p_2}_{[L]_0(\mathbb{R})}\left\|[|\nabla|\langle\nabla\rangle^{-1}_n - 1]\widehat{U}_\infty\right\|_{[L]_0(\mathbb{R})} \\ &\lesssim \|\widehat{U}_\infty\|^{p_2}_{[L]_0(\mathbb{R})}\|\langle\nabla/h_n\rangle^{-2}\widehat{U}_\infty\|_{[L]_0(\mathbb{R})} \to 0,\end{aligned} \tag{5-86}$$

since $\widehat{U}_\infty \in [H]^\bullet_2 \cap [W]^\bullet_2 \subset [L]_0$ by the homogeneous version of Lemma 4.3(1).

If $d \ge 5$, we introduce a new exponent

$$G := \frac{d-2}{d+2}\left(\frac{1}{d+1}, \frac{d+3}{2(d+1)}, 0\right). \tag{5-87}$$

Then $\mathrm{reg}^0(G) = 1$, $\mathrm{str}^0(G) < 0$ and

$$(2^\star - 1)G = W^{*(1)} - \frac{(1,0,1)}{2}. \tag{5-88}$$

Hence

$$\begin{aligned}&\|f'(u_{(n)}) - f'(u_{\langle n\rangle})\|_{[W^{*(1)}]_2(I)} \\ &\qquad\lesssim \|f'(u_{(n)}) - f'(u_{\langle n\rangle})\|_{[W^{*(1)}]^\bullet_2(\mathbb{R})} + |I|^{1/2}\|f'(u_{(n)}) - f'(u_{\langle n\rangle})\|_{[(2^\star-1)G]_0(I)},\end{aligned} \tag{5-89}$$

where the first term on the right is dominated by (the homogeneous version of (5-83)–(5-84))

$$\begin{aligned}&\|u_{\langle n\rangle}\|^{p_2}_{[M^\sharp_\varepsilon]_0(\mathbb{R})}\|u_{(n)} - u_{\langle n\rangle}\|_{[W_\varepsilon]^\bullet_2(\mathbb{R})} + \|u_{(n)} - u_{\langle n\rangle}\|^\theta_{[M^\sharp_\varepsilon]_0(\mathbb{R})}\|(u_{\langle n\rangle}, u_{(n)})\|^{p_2-\theta}_{[W_\varepsilon]^\bullet_2(\mathbb{R})} \\ &\qquad\lesssim \|\widehat{U}_\infty\|^{p_2}_{[M^\sharp_\varepsilon]_0(\mathbb{R})}\|\langle\nabla/h_n\rangle^{-2}\widehat{U}_\infty\|_{[W_\varepsilon]^\bullet_2(\mathbb{R})} + \|\langle\nabla/h_n\rangle^{-2}\widehat{U}_\infty\|^\theta_{[M^\sharp_\varepsilon]_0(\mathbb{R})}\|\widehat{U}_\infty\|^{p_2-\theta}_{[W_\varepsilon]^\bullet_2(\mathbb{R})},\end{aligned} \tag{5-90}$$

where $\theta := \min(p_2, 1)$. The right-hand side goes to 0, since $\widehat{U}_\infty \in [H]^\bullet_2 \cap [W_\varepsilon]^\bullet_2 \subset [M^\sharp_\varepsilon]_0$ by the homogeneous version of Lemma 4.3(1). Similarly, the last term in (5-89) is bounded by

$$\|u_{\langle n\rangle}\|^{p_2}_{[G]_0(\mathbb{R})}\|u_{(n)} - u_{\langle n\rangle}\|_{[G]_0(\mathbb{R})} \sim \|\widehat{U}_\infty\|^{p_2}_{[G]_0(\mathbb{R})}\|\langle\nabla/h_n\rangle^{-2}\widehat{U}_\infty\|_{[G]_0(\mathbb{R})} \to 0. \tag{5-91}$$

Thus it suffices to show

$$\Big\|f'\Big(\sum_{j<k} u^j_{\langle n\rangle}\Big) - \sum_{j<k} f'(u^j_{\langle n\rangle})\Big\|_{ST^*(I)} \to 0. \tag{5-92}$$

Now we define $\widehat{U}^j_{n,R}$ for any $R \gg 1$ by

$$\widehat{U}^j_{n,R}(t,x) = \chi_R(t,x)\widehat{U}^j_\infty(t,x)\prod\{(1-\chi_{h^{j,l}_n R})(t-t^{j,l}_n, x-x^{j,l}_n) \mid 1 \le l < k,\ h^l_n R < h^j_n\}, \tag{5-93}$$

where χ_R and $(t^{j,l}_n, x^{j,l}_n, h^{j,l}_n)$ are as defined respectively in (1-23) and (5-21). Then $\widehat{U}^j_{n,R}$ is uniformly bounded in $[H]^\bullet_2(\mathbb{R}) \cap [W]^\bullet_2(\mathbb{R})$, and

$$\widehat{U}^j_{n,R} \to \chi_R\widehat{U}^j_\infty \quad \text{in } [M^\sharp]_0(\mathbb{R}) \text{ as } n \to \infty,$$

because either $h_n^{j,l} \to 0$ or $|t_n^{j,l}| + |x_n^{j,l}| \to \infty$ by the orthogonality (5-5). Then by the homogeneous version of Lemma 4.3(2), it converges also in $[L]_0(\mathbb{R})$ (if $d \le 4$), $[W_\varepsilon]_2^\bullet(\mathbb{R})$ and $[M_\varepsilon^\sharp]_0(\mathbb{R})$. Moreover, we have $\chi_R \widehat{U}_\infty^j \to \widehat{U}_\infty^j$ as $R \to \infty$ in the same spaces.

Hence we may replace $u_{\langle n\rangle}^j$ by

$$u_{\langle n\rangle,R}^j := h_n^j T_n^j \widehat{U}_{n,R}^j((t-t_n^j)/h_n^j),$$

and then we get the desired result, since $\{\operatorname{supp}_{(t,x)} u_{\langle n\rangle,R}^j\}_{j<k}$ are mutually disjoint for large n, and so

$$f'\Big(\sum_{j<k} u_{\langle n\rangle,R}^j\Big) = \sum_{j<k} f'(u_{\langle n\rangle,R}^j), \tag{5-94}$$

which concludes the proof of (5-66). □

The next lemma is the conclusion of this section.

Lemma 5.6. *Assume that f satisfies* (1-36). *Let u_n be a sequence of local solutions of NLKG around $t = 0$ in $\mathcal{K}^+$ satisfying $\overline{\lim}_{n\to\infty} E(u_n) < m$. Suppose that in its nonlinear profile decomposition* (5-58), *every nonlinear profile $\vec{U}_\infty^j$ has finite global Strichartz and energy norms*, *i.e.*

$$\|\widehat{U}_\infty^j\|_{ST_\infty^j(\mathbb{R})} + \|\vec{U}_\infty^j\|_{L_t^\infty L_x^2(\mathbb{R})} < \infty. \tag{5-95}$$

Then u_n is bounded for large n in the Strichartz and the energy norms, *i.e.*

$$\overline{\lim_{n\to\infty}} \|u_n\|_{ST(\mathbb{R})} + \|\vec{u}_n\|_{L_t^\infty L_x^2(\mathbb{R})} < \infty. \tag{5-96}$$

Proof. We will apply the perturbation lemma to $u_{(n)}^{<k} + w_n^k$ as an approximate solution. First observe that

$$\|\vec{u}_n(0) - \vec{u}_{(n)}^{<k}(0) - w_n^k(0)\|_{L_x^2} \le \sum_{j<k} \|\vec{v}_n^j(0) - \vec{u}_{(n)}^j(0)\|_{L_x^2} = o(1) \tag{5-97}$$

and

$$\|\vec{u}_n(0)\|_{L^2}^2 = \|\vec{v}_n\|_{L_x^2}^2 \ge \sum_{j<k} \|\vec{v}_n^j\|_{L_x^2}^2 + o(1) = \sum_{j<k} \|\vec{u}_{(n)}^j(0)\|_{L_x^2}^2 + o(1), \tag{5-98}$$

where $o(1) \to 0$ as $n \to \infty$. Hence except for a finite set $J \subset \mathbb{N}$, the energy of $u_{(n)}^j$ with $j \notin J$ is smaller than the iteration threshold, which implies

$$\|u_{(n)}^j\|_{ST(\mathbb{R})} \lesssim \|\vec{u}_{(n)}^j(0)\|_{L_x^2} \quad (j \notin J). \tag{5-99}$$

Combining (5-65), (5-64), (5-99) and (5-98), we obtain, for any finite interval I,

$$\sup_k \overline{\lim_{n\to\infty}} \|u_{(n)}^{<k}\|_{ST(I)}^2 \lesssim \sum_{j\in J} \|\widehat{U}_\infty^j\|_{ST_\infty^j}^2 + \overline{\lim_{n\to\infty}} \|\vec{u}_n(0)\|_{L_x^2}^2 < \infty. \tag{5-100}$$

The equation of $u_{(n)}^{<k}$ is given by

$$eq(u_{(n)}^{<k}) = \sum_{j<k} \big(\langle\nabla\rangle - \langle\nabla\rangle_\infty^j\big)\vec{u}_{(n)}^j + f'\big(u_{(n)}^{<k}\big) - \sum_{j<k} f'\big(u_{\langle n\rangle}^j\big), \tag{5-101}$$

where $u^j_{\langle n\rangle} = (\langle\nabla\rangle^j_\infty)^{-1}\langle\nabla\rangle u^j_{(n)}$ as before. The nonlinear part goes to 0 by (5-66), while the linear part vanishes if $h^j_\infty = 1$, and is dominated if $h^j_\infty = 0$ by

$$\begin{aligned}\|(\langle\nabla\rangle - |\nabla|)\vec{u}^j_{(n)}\|_{L^1_t L^2_x(I)} &\lesssim |I|\,\|\langle\nabla\rangle^{-1}\vec{u}^j_{(n)}\|_{L^\infty_t L^2_x(\mathbb{R})}\\ &\sim |I|\,\|\langle\nabla/h^j_n\rangle^{-1}\vec{U}^j_\infty\|_{L^\infty_t L^2_x(\mathbb{R})} \to 0 \quad (n\to\infty),\end{aligned} \tag{5-102}$$

by continuity in t for bounded t, and by the scattering of $\widehat{U}^j_\infty$ for $|t|\to\infty$, which follows from $\|\widehat{U}^j_\infty\|_{[W]^\bullet_2(\mathbb{R})} < \infty$. Hence Lemma 4.4 gives for any 1-admissible Z

$$\sup_k \varlimsup_{n\to\infty} \|u^{<k}_{(n)}\|_{[Z]_2(\mathbb{R})} < \infty. \tag{5-103}$$

On the other hand, by Lemma 4.3 we can extend the smallness of w^k_n from $L^\infty_t B^s_{\infty,\infty}$ to the other spaces that we need for the nonlinear difference estimates, those being $[S]_0$, $[L]_0$, $[X]_2$, $[H_\varepsilon]_0$, $[M^\sharp_\varepsilon]_0$, and $[W_\varepsilon]_2$, depending on d and f. In addition, in the exponential case (1-29), Lemmas 5.3 and 2.11 imply that $u^{<k}_{(n)}$ and w^k_n are both in the subcritical regime for the Trudinger–Moser inequality. Putting them together with the above bounds on $u^{<k}_{(n)}$ in the nonlinear difference estimates (4-61)–(4-64) or (5-82)–(5-84), we get

$$\lim_{k\to K} \varlimsup_{n\to\infty} \|f'(u^{<k}_{(n)} + w^k_n) - f'(u^{<k}_{(n)})\|_{ST^*(I)} = 0, \tag{5-104}$$

and so

$$\lim_{k\to K} \varlimsup_{n\to\infty} \|eq(u^{<k}_{(n)} + w^k_n)\|_{ST^*(I)} = 0. \tag{5-105}$$

Hence for k sufficiently close to K and n large enough, the true solution u_n and the approximate solution $u^{<k}_{(n)} + w^k_n$ satisfy all the assumptions of the perturbation Lemma 4.5. Hence u_n is bounded in global Strichartz norms for large n. □

6. Extraction of a critical element

In this section, we prove that if uniform global Strichartz bound fails strictly below the variational threshold m, then we have a global solution in $\mathcal{K}^+$ with infinite Strichartz norm and with the minimal energy, which is called *a critical element*.

Let $E^\star$ be the threshold for the uniform Strichartz bound. More precisely,

$$E^\star := \sup\{A > 0 \mid S(A) < \infty\}, \tag{6-1}$$

where $S(A)$ denotes the supremum of $\|u\|_{ST(I)}$ for any strong solution u in $\mathcal{K}^+$ on any interval I satisfying $E(u) \le A$.

The small energy scattering tells us $E^\star > 0$, and the presence of the ground state tells us $E^\star \le m$, at least in the subcritical case, and also in the other cases if we allow complex-valued solutions, because the stationary solutions with different masses yield standing wave solutions of the original NLKG. Anyway, we are going to prove $E^\star \ge m$ by contradiction.

We remark that there is an alternative threshold:

$$E^\star_{FS} := \sup\left\{A > 0 \;\middle|\; \begin{array}{l}\text{if } u \text{ is a solution in } \mathcal{K}^+ \text{ of NLKG}\\ \text{with } E(u) \le A, \text{ then } \|u\|_{ST(\mathbb{R})} < \infty\end{array}\right\}. \tag{6-2}$$

Obviously $E^\star \le E^\star_{FS}$. Kenig and Merle [2008] chose this definition. The advantage of using $E^\star$ is that $E^\star \ge m$ implies uniform bound on the global Strichartz norms below m, which is very important in applications where we want to perturb the equation.

The next lemma is the conclusion of this section.

Lemma 6.1. *Assume that f satisfies* (1-36), *and let u_n be a sequence of solutions of NLKG in $\mathcal{H}^+$ on $I_n \subset \mathbb{R}$ satisfying*

$$E(u_n) \to E^\star < m, \quad \|u_n\|_{ST(I_n)} \to \infty \quad (n \to \infty). \tag{6-3}$$

Then there exists a global solution u_* of NLKG in $\mathcal{H}^+$ satisfying

$$E(u_*) = E^\star, \quad \|u_*\|_{ST(\mathbb{R})} = \infty. \tag{6-4}$$

In addition, there are a sequence $(t_n, x_n) \in \mathbb{R}\times\mathbb{R}^d$ and $\varphi \in L^2(\mathbb{R}^d)$ such that along some subsequence,

$$\|\vec{u}_n(0,x) - e^{-i\langle\nabla\rangle t_n}\varphi(x-x_n)\|_{L^2_x} \to 0. \tag{6-5}$$

We call such a global solution u_* *a critical element*. Observe that by the definition of $E^\star$, we can find such a sequence u_n, once we have $E^\star < m$.

Proof. We can translate u_n in t so that $0 \in I_n$ for all n. Then we consider the linear and nonlinear profile decompositions of u_n, using Lemma 5.1 in the H^1 critical case (1-28) and Corollary 5.2 in the subcritical and exponential cases.

$$\begin{aligned} &e^{i\langle\nabla\rangle t}\vec{u}_n(0) = \sum_{j<k}\vec{v}^j_n + \vec{w}^k_n, \quad \vec{v}^j_n = e^{i\langle\nabla\rangle(t-t^j_n)}T^j_n\varphi^j, \\ &u^{<k}_{(n)} = \sum_{j<k} u^j_{(n)}, \quad \vec{u}^j_{(n)} = T^j_n \vec{U}^j_\infty((t-t^j_n)/h^j_n), \\ &\|\vec{v}^j_n(0) - \vec{u}^j_{(n)}(0)\|_{L^2_x} \to 0 \quad (n\to\infty). \end{aligned} \tag{6-6}$$

Lemma 5.6 precludes that all the nonlinear profiles $\vec{U}^j_\infty$ have finite global Strichartz norm. On the other hand, every solution of NLKG in $\mathcal{H}^+$ with energy less than $E^\star$ has global finite Strichartz norm by the definition of $E^\star$. Hence by Lemma 5.3 we deduce that there is only one profile i.e. $K = 1$, and moreover

$$\widetilde{E}(\vec{u}^0_{(n)}) = E^\star, \quad \vec{u}^0_{(n)}(0) \in \widetilde{\mathcal{H}}^+, \quad \|\widehat{U}^0_\infty\|_{ST^0_\infty(\mathbb{R})} = \infty, \quad \lim_{n\to\infty}\|\vec{w}^1_n\|_{L^\infty_t L^2_x} = 0. \tag{6-7}$$

If $h^0_n \to 0$ in the critical case, then $\widehat{U}^0_\infty = |\nabla|^{-1}\operatorname{Re}\vec{U}^0_\infty$ solves the massless equation

$$(\partial_t^2 - \Delta)\widehat{U}^0_\infty = f'(\widehat{U}^0_\infty), \tag{6-8}$$

and satisfies

$$E^0(\widehat{U}^0_\infty) = E^\star < m = J^{(0)}(Q), \quad K^w(\widehat{U}^0_\infty(0)) \ge 0, \quad \|\widehat{U}^0_\infty\|_{[W]^\bullet_2} = \infty, \tag{6-9}$$

where Q is the massless ground state and K^w is the massless version of K. However, there is no such solution, by [Kenig and Merle 2008].[5] Hence $h^0_n \equiv 1$ in all cases, and we obtain (6-5).

[5] That reference is restricted to the dimensions $d \le 5$ for simplicity of the perturbation argument, but the elimination of critical elements works in any higher dimensions.

Hence $h_n^0 \equiv 1$ in all cases, and we obtain (6-5).

It remains to prove that $\widehat{U}_\infty^0 = \langle\nabla\rangle^{-1}\operatorname{Re}\vec{U}_\infty^0$ is a global solution. Suppose not. Then we can choose a sequence $t_n \in \mathbb{R}$ approaching the maximal existence time. Since the sequence of solutions $\widehat{U}_\infty^0(t+t_n)$ satisfies the assumption of this lemma, we may apply the above argument to it. In particular, from (6-5) we obtain

$$\|\vec{U}_\infty^0(t_n) - e^{-i\langle\nabla\rangle t_n'}\psi(x-x_n')\|_{L_x^2} \to 0, \tag{6-10}$$

for some $\psi \in L_x^2$ and another sequence $(t_n', x_n') \in \mathbb{R}\times\mathbb{R}^d$. Let $\vec{v} := e^{i\langle\nabla\rangle t}\psi$. Since it is a free solution, for any $\varepsilon > 0$ there is $\delta > 0$ such that for any interval I satisfying $|I| \le 2\delta$, we have $\|\langle\nabla\rangle^{-1}\vec{v}\|_{ST(I)} \le \varepsilon$, where $ST = [W]_2 \cap [K]_2$ as in (5-59). Then (6-10) implies that

$$\overline{\lim_{n\to\infty}}\, \|\langle\nabla\rangle^{-1}e^{i\langle\nabla\rangle t}\vec{U}_\infty^0(t_n)\|_{ST(-\delta,\delta)} \le \varepsilon. \tag{6-11}$$

If $\varepsilon > 0$ is small enough, this implies that the solution $\widehat{U}_\infty^0$ exists on $(t_n-\delta, t_n+\delta)$, by the iteration argument, for large n. This contradicts the choice of t_n. Hence $\widehat{U}_\infty^0$ is global and so a critical element. □

7. Extinction of the critical element

In this section, we prove that the critical element can not exist by deriving a contradiction from a few properties of it. The main idea follows [Kenig and Merle 2006; 2008]. Let u_c be a critical element given by Lemma 6.1. Since NLKG is symmetric in t, we may assume that $\|u_c\|_{ST(0,\infty)} = \infty$. We call such u a *forward critical element*. Note that since the critical element is in $\mathcal{K}^+$, we have $E^Q(u;t) \sim E(u)$ uniformly, by Lemma 2.10.

Compactness. First we show that the trajectory of a forward critical element is precompact for positive time in the energy space modulo spatial translations.

Lemma 7.1. *Assume that f satisfies* (1-36), *and let u_c be a forward critical element. Then there exists $c : (0,\infty) \to \mathbb{R}^d$ such that the set*

$$\{(u,\dot{u})(t, x-c(t)) \mid 0 < t < \infty\} \tag{7-1}$$

is precompact in $H^1(\mathbb{R}^d)\times L^2(\mathbb{R}^d)$.

Proof. The proof in [Kenig and Merle 2008] can be adapted verbatim, but we give a sketch for the sake of completeness. Recall the convention $u \leftrightarrow \vec{u}$ defined on page 427.

It suffices to prove precompactness of $\{\vec{u}(t_n)\}$ in L_x^2 for any $t_1, t_2, \dots > 0$. If t_n converges, then it is trivial from the continuity in t. Hence we may assume that $t_n \to \infty$. Applying Lemma 6.1 to the sequence of solutions $u(t+t_n)$, we get another sequence $(t_n', x_n') \in \mathbb{R}^{1+d}$ and $\varphi \in L^2$ such that

$$\vec{u}(t_n, x) - e^{-i\langle\nabla\rangle t_n'}\varphi(x-x_n') \to 0 \text{ in } L_x^2 \quad (n\to\infty). \tag{7-2}$$

If $t_n' \to -\infty$, then we have

$$\|e^{i\langle\nabla\rangle t}\vec{u}(t_n)\|_{ST(0,\infty)} = \|e^{i\langle\nabla\rangle t}\varphi\|_{ST(-t_n',\infty)} + o(1) \to 0, \tag{7-3}$$

so that we can solve NLKG of u for $t > t_n$ with large n globally by iteration with small Strichartz norms, contradicting its forward criticality.

If $t'_n \to +\infty$, then we have

$$\|e^{i\langle\nabla\rangle t}\vec{u}(t_n)\|_{ST(-\infty,0)} = \|e^{i\langle\nabla\rangle t}\varphi\|_{ST(-\infty,-t'_n)} + o(1) \to 0, \tag{7-4}$$

so that we can solve NLKG of u for $t < t_n$ with large n with diminishing Strichartz norms, which implies $u = 0$ by taking the limit, a contradiction.

Thus t'_n is precompact, so is $\vec{u}(t_n, x + x'_n)$ in L^2_x by (7-2). □

As a consequence, the energy of u stays within a fixed radius for all positive time, modulo arbitrarily small rest. More precisely, we define the exterior energy by

$$E_{R,c}(u;t) = \int_{|x-c|\geq R} |u_t|^2 + |\nabla u|^2 + |u|^2 + |f(u)| + |uf'(u)|dx, \tag{7-5}$$

for any $R > 0$ and $c \in \mathbb{R}^d$. Then we have

Corollary 7.2. *Let u be a forward critical element. Then for any $\varepsilon > 0$, there exist $R_0(\varepsilon) > 0$ and $c(t) : (0,\infty) \to \mathbb{R}^d$ such that at any $t > 0$ we have*

$$E_{R_0,c(t)}(u;t) \leq \varepsilon E(u). \tag{7-6}$$

Zero momentum and non-propagation. Next we observe that the critical element can not move with any positive speed in the sense of energy. For that we first need to see that the (conserved) momentum

$$P(u) := \int_{\mathbb{R}^d} u_t \nabla u dx \in \mathbb{R}^d \tag{7-7}$$

is zero for any critical element u.

Lemma 7.3. *For any critical element u, we have $P(u) = 0$.*

Proof. For $j = 1, \dots, d$ and $\lambda \in \mathbb{R}$, we define the operator L_j^λ of Lorentz transformation:

$$\begin{gathered} L_j^\lambda u(x_0, \dots, x_d) = u(y_0, \dots, y_d), \\ y_0 = x_0 \cosh\lambda + x_j \sinh\lambda, \quad y_j = x_0 \sinh\lambda + x_j \cosh\lambda, \quad y_k = x_k \ (k \neq 0, j). \end{gathered} \tag{7-8}$$

Then $L_j^\alpha L_j^\beta = L_j^{\alpha+\beta}$. Since $\partial_\lambda y_0 = y_j$ and $\partial_\lambda y_j = y_0$, we have

$$\partial_\lambda L_j^\lambda u = L_j^\lambda[(x_j\partial_t + t\partial_j)u]. \tag{7-9}$$

Also we have

$$\begin{aligned} \partial_t L_j^\lambda &= L_j^\lambda(s\partial_t + c\partial_j), & \partial_{tt} L_j^\lambda &= L_j^\lambda(s^2\partial_{tt} + 2sc\partial_{tj} + c^2\partial_{jj}), \\ \partial_j L_j^\lambda &= L_j^\lambda(c\partial_t + s\partial_j), & \partial_{jj} L_j^\lambda &= L_j^\lambda(c^2\partial_{tt} + 2sc\partial_{tj} + s^2\partial_{jj}), \end{aligned} \tag{7-10}$$

where $s := \sinh\lambda$ and $c := \cosh\lambda$. In particular $[\partial_t^2 - \Delta, L_j^\lambda] = 0$, and so L_j^λ maps global solutions to themselves. For the space-time norm, we have

$$\iint L_j^\lambda v \, dt \, dx_j = \iint v \left|\begin{pmatrix} c & s \\ s & c \end{pmatrix}\right| dt \, dx_j = \iint v \, dt \, dx_j; \tag{7-11}$$

hence L_j^λ preserves all $L^p_{t,x}(\mathbb{R}^{1+d})$ norm. For any solution u, we have

$$\begin{aligned}\partial_\lambda^0 E(L_j^\lambda u) &= \langle u_t \mid \partial_\lambda^0 \partial_t L_j^\lambda u\rangle + \langle \nabla u \mid \partial_\lambda^0 \nabla L_j^\lambda u\rangle + \langle u - f'(u) \mid \partial_\lambda^0 L_j^\lambda u\rangle \\ &= \langle u_t \mid x_j u_{tt} + t u_{tj} + u_j\rangle + \langle u_k \mid x_j u_{kt} + t u_{kj} + \delta_{kj} u_t\rangle + \langle u - f'(u) \mid x_j u_t + t u_j\rangle \\ &= \langle x_j u_t \mid \Delta u\rangle + 2\langle u_t \mid u_j\rangle - \langle x_j u_{kt} \mid u_k\rangle = \langle u_t \mid u_j\rangle = P(u), \end{aligned} \tag{7-12}$$

where $\partial_\lambda^0 := \partial_\lambda|_{\lambda=0}$. If $P_j(u) \neq 0$ for some j, then we obtain another global solution $L_j^\lambda u$, which has smaller energy and infinite Strichartz norm. It also belongs to $\mathcal{K}^+$, by continuity. More precisely, the continuity of $L_j^\lambda u$ in λ in the energy space easily follows from the local wellposedness if u has compactly supported initial data. Then the original solution is approximated by smooth cut-off using the finite propagation property. Thus we obtain another critical element with less energy, a contradiction. Hence $P(u) = 0$. □

Next we see stillness of critical elements in terms of the energy propagation. For any $R > 0$, we define the localized center of energy $X_R(t) \in \mathbb{R}^d$ by

$$X_R(u;t) := \int \chi_R(x) x e(u)(t,x)\,dx, \tag{7-13}$$

where χ_R is as defined in (1-23), and $e(u)$ denote the energy density of u, namely

$$e(u) = (|u_t|^2 + |\nabla u|^2 + |u|^2)/2 - f(u). \tag{7-14}$$

From the energy identity $\dot{e}(u) = \nabla\cdot(u_t \nabla u)$, we get for any solution u

$$\frac{d}{dt} X_R(u;t) = -dP(u) + \int [d(1-\chi_R(x)) + (r\partial_r)\chi_R(x)] u_t \nabla u. \tag{7-15}$$

If u is a critical element, the first term disappears by the above lemma, so we have

$$\left|\frac{d}{dt} X_R(u;t)\right| \lesssim E_{R,0}(u;t). \tag{7-16}$$

Moreover, since u is in $\mathcal{K}^+$, by Lemma 2.12 there exists $\delta_0 \in (0,1)$ such that

$$K_{1,0}(u(t)) \geq \delta_0 \|u(t)\|^2_{H^1} \quad \text{for all } t \in \mathbb{R}. \tag{7-17}$$

Lemma 7.4. *Let u be a forward critical element, and let $R_0(\varepsilon) > 0$, $c(t) \in \mathbb{R}^d$ and $\delta_0 > 0$ be as in* (7-6) *and* (7-17). *If $0 < \varepsilon \ll \delta_0$ and $R \gg R_0(\varepsilon)$ then we have*

$$|c(t) - c(0)| \leq R - R_0(\varepsilon), \tag{7-18}$$

for $0 < t < t_0$ till some $t_0 \gtrsim \delta_0 R/\varepsilon$.

Proof. By translation in x, we may assume that $c(0) = 0$. Let t_0 be the final time for the above property

$$t_0 = \inf\{t > 0 \mid |c(t)| \geq R - R_0\}. \tag{7-19}$$

Then the finite speed of propagation implies that $t_0 > 0$. For any $0 < t < t_0$ we have $|c(t)| \le R - R_0$, hence by (7-6) we have $E_{R,0} \le \varepsilon E(u)$, and so by (7-16) we get

$$\left| \frac{d}{dt} X_R(u;t) \right| \lesssim \varepsilon E(u). \tag{7-20}$$

Next we expand it around c:

$$c(t) \cdot X_R(u;t) = |c(t)|^2 \int \chi_R(x) e(u)\, dx + \int \chi_R(x) c \cdot (x - c) e(u)\, dx, \tag{7-21}$$

where the first term on the right is bounded from below by

$$\begin{aligned} E(u) - \int (1 - \chi_R(x)) e(u)\, dx &\ge \|\dot u(t)\|_{L_x^2}^2/2 + K_{1,0}(u(t)) - C E_{R,0}(t) \\ &\ge \delta_0 E(u) - C\varepsilon E(u) \gtrsim \delta_0 E(u), \end{aligned} \tag{7-22}$$

since $\varepsilon \ll \delta_0$. The second term of (7-21) is dominated by splitting the integral into $|x - c| \le R_0$ and $|x - c| \ge R_0$. In the interior it is bounded by using the energy bound, and in the exterior it is bounded by using (7-6). Thus we obtain

$$\left| \int \chi_R(x) c \cdot (x - c) e(u)\, dx \right| \lesssim (R_0 + R\varepsilon) E(u) |c|. \tag{7-23}$$

In the same way we have $|X_R(u;0)| \lesssim (R_0 + R\varepsilon) E(u)$, since $c(0) = 0$. Thus we get

$$\delta_0 E(u) |c(t)| \lesssim (R_0 + R\varepsilon + \varepsilon t) E(u), \tag{7-24}$$

and sending $t \to t_0$, we get $\delta_0 R \lesssim \varepsilon t_0$. □

Dispersion and contradiction. Finally we use the localized virial identity to see dispersion of the critical element, which will contradict the above non-propagation property. For any $R > 0$, we define the localized virial $V_R(u;t) \in \mathbb{R}$ by

$$V_R(u;t) := \langle \chi_R(x) u_t \mid (x \cdot \nabla + \nabla \cdot x) u \rangle, \tag{7-25}$$

where χ_R is as defined in (1-23). Then we have for any solution u,

$$\begin{aligned} \frac{d}{dt} V_R(u;t) = &- \int \chi_R(x) [2|\nabla u|^2 - d(D-2) f(u)] + \frac{d}{2} |u|^2 \Delta \chi_R(x)\, dx \\ &- \int r \partial_r \chi_R(x) \left[|u_t|^2 + 2|u_r|^2 - |\nabla u|^2 - |u|^2 + 2f(u) \right] dx \\ \le &-K_{d,-2}(u(t)) + C E_{R,0}(u;t). \end{aligned} \tag{7-26}$$

If u is a critical element, then $u \in \mathscr{K}^+$ and hence by Lemma 2.12, there exists $\delta_2 \in (0,1)$ such that

$$K_{d,-2}(u(t)) \ge \delta_2 \|\nabla u(t)\|_{L_x^2}^2 \tag{7-27}$$

for all $t > 0$. Thus we obtain, integrating in t,

$$V_R(u;t_0) \le V_R(u;0) - \delta_2 \int_0^{t_0} \|\nabla u(t)\|_{L_x^2}^2\, dt + C\varepsilon E(u) t_0. \tag{7-28}$$

Now by the compactness Lemma 7.1, we have:

Lemma 7.5. *Let u be a forward critical element. Then for any $\varepsilon > 0$ there exists $C > 0$ such that*

$$\|u(t)\|_{L^2_x}^2 \le C\|\nabla u(t)\|_{L^2_x}^2 + \varepsilon\|\dot u(t)\|_{L^2_x}^2, \tag{7-29}$$

for all $t > 0$.

Proof. Otherwise there exists a sequence $t_n > 0$ such that

$$\|u(t_n)\|_{L^2_x}^2 > n\|\nabla u(t_n)\|_{L^2_x}^2 + \varepsilon\|\dot u(t_n)\|_{L^2_x}^2. \tag{7-30}$$

Since u is L^2_x bounded, it follows that $\|\nabla u(t_n)\|_{L^2_x} \to 0$. Then Lemma 7.1 implies that, after passing to a subsequence, $u(t_n) \to 0$ strongly in H^1_x, then the above inequality implies that $\dot u(t_n) \to 0$ too. Hence $E^Q(u; t_n) \to 0$, which contradicts the energy equivalence, Lemma 2.10. □

Multiplying the equation with u, and then applying the above lemma with $\varepsilon = \frac{1}{4}$, we obtain

$$\partial_t\langle u \mid \dot u\rangle = \int_{\mathbb{R}^d} |\dot u|^2 - |\nabla u|^2 - |u|^2 + Df(u)\,dx \ge \int_{\mathbb{R}^d} |\dot u|^2/2 + |u|^2 - C|\nabla u|^2 dx, \tag{7-31}$$

with some $C > 0$. Hence

$$\int_0^{t_0} \|\dot u\|_{L^2_x}^2 + \|u\|_{L^2_x}^2 dt \lesssim E(u) + \int_0^{t_0} \|\nabla u\|_{L^2_x}^2 dt, \tag{7-32}$$

and so

$$t_0 E(u) \le \int_0^{t_0} E^Q(u; t)\,dt \lesssim E(u) + \int_0^{t_0} \|\nabla u\|_{L^2_x}^2 dt. \tag{7-33}$$

Now we choose positive $\varepsilon \ll \delta_2\delta_0$ and $R \gg R_0(\varepsilon)$. Then by Lemma 7.4 there exists $t_0 \sim \delta_0 R/\varepsilon$ such that $E_{R,0}(u; t) \le \varepsilon E(u)$ for $0 < t < t_0$. Then from (7-28) and (7-33), we have

$$-V_R(u; t_0) + V_R(u; 0) \gtrsim [\delta_2 t_0 - C\varepsilon t_0 - C]E(u) \gtrsim \delta_2 t_0 E(u) \sim \frac{\delta_2\delta_0 R}{\varepsilon} E(u), \tag{7-34}$$

while the left-hand side is dominated by $RE(u)$ — a contradiction when $\varepsilon/\delta_2\delta_0$ is small enough. □

Appendix: The range of scaling exponents

In Section 2, we have shown that $m_{\alpha,\beta}$ in (1-17) is positive and achieved (after modification of the mass in the critical and exponential cases) if (α, β) satisfies (1-16). Here we see that it is also necessary, modulo the obvious symmetry $(\alpha, \beta) \to (-\alpha, -\beta)$. For simplicity, we consider only the pure power nonlinearity.

Proposition A.1. *Assume that neither $(\alpha, \beta) \in \mathbb{R}^2$ nor $(-\alpha, -\beta)$ satisfies (1-16). There exists $q \in (2_\star, 2^\star)$ such that $m_{\alpha,\beta} = -\infty$ for $f(\varphi) = |\varphi|^q$.*

Proof. By symmetry with respect to $(\alpha, \beta) \to (-\alpha, -\beta)$, we may assume that $\beta > 0$ and $\bar\mu = 2\alpha + d\beta > 0$.

First we consider the case $\alpha < 0$ and $\underline{\mu} > 0$, which implies that $d \ge 2$. Let $(2_\star, 2^\star) \ni q = 2 + p$, then we have

$$\alpha p + \bar\mu \ge d\underline{\mu}/(d-2) > 0. \tag{A-1}$$

Decompose $K(\varphi)$ by setting

$$K = K_1 + K_2, \quad K_1(\varphi) = \underline{\mu}\frac{\|\nabla\varphi\|_{L^2}^2}{2}, \quad K_2(\varphi) = \bar{\mu}\frac{\|\varphi\|_{L^2}^2}{2} - (\alpha p + \bar{\mu})F(\varphi). \tag{A-2}$$

Suppose that $0 \neq \varphi \in H^1(\mathbb{R}^d)$ satisfies $K_2(\varphi) = 0$. If there is no such φ, then K is positive definite and the minimization set in (1-17) becomes empty. Let $1 < \nu \to 1+0$. Then

$$0 > K_2(\nu\varphi) \to K_2(\varphi) = 0, \quad K_1(\nu\varphi) \to K_1(\varphi) > 0. \tag{A-3}$$

Now let $\lambda(\nu) > 0$ solve

$$0 = K(\nu\varphi(x/\lambda)) = \lambda^{d-2}K_1(\nu\varphi) + \lambda^d K_2(\nu\varphi); \tag{A-4}$$

in other words $\lambda(\nu) = [-K_2(\nu\varphi)/K_1(\nu\varphi)]^{1/2}$. Then $\lambda(\nu) \to \infty$ as $\nu \to 1+0$ due to (A-3). Since

$$\bar{\mu}J(\psi) = K(\psi) + \beta\|\nabla\psi\|_{L^2}^2 + \alpha p F(\psi), \tag{A-5}$$

we obtain

$$\bar{\mu}J(\nu\varphi(x/\lambda)) = \beta\nu^2\lambda^{d-2}\|\nabla\varphi\|_{L^2}^2 + \alpha p\lambda^d F(\nu\varphi) \to -\infty, \tag{A-6}$$

which implies that $m = -\infty$.

Next, if $\bar{\mu} = 0 > \alpha$, which implies $d \geq 2$, then for any nonzero $\varphi \in H^1(\mathbb{R}^d)$ satisfying $K(\varphi) = 0$ we have

$$K(\varphi(x/\lambda)) = \lambda^d K(\varphi) = 0, \tag{A-7}$$

and similarly as above,

$$J(\varphi(x/\lambda)) = O(-\lambda^d) \to \infty \quad \text{as } \lambda \to \infty.$$

Finally consider the case $\underline{\mu} < 0 < \bar{\mu}$. Then $\alpha p + 2\beta = 0$ has a solution $p \in (4/d, 2^\star - 2)$. Since $\alpha p + \bar{\mu} = \alpha p + 2\beta + \underline{\mu}$, there exists $p \in (4/d, 2^\star - 2)$ such that

$$\alpha p + \bar{\mu} < 0 < \alpha p + 2\beta. \tag{A-8}$$

Then $K^N(\varphi) = -(\alpha p + \bar{\mu})F(\varphi)$ is positive and so for any $\varphi \in H^1(\mathbb{R}^d)$, $K(\nu\varphi) \geq 0$ if $\nu \gg 1$. Since the kinetic term in K is negative, there exists $\xi(\nu) \in \mathbb{R}^d$ such that $K(e^{i\xi x}\nu\varphi) = 0$. Since

$$-\underline{\mu}J(\psi) = -K(\psi) + 2\beta\frac{\|\varphi\|_{L^2}^2}{2} - (\alpha p + 2\beta)F(\psi), \tag{A-9}$$

we obtain

$$-\underline{\mu}J(e^{i\xi x}\nu\varphi) = 2\beta\nu^2\frac{\|\varphi\|_{L^2}^2}{2} - (\alpha p + 2\beta)F(\nu\psi) \to -\infty, \tag{A-10}$$

which implies that $m = -\infty$. □

The above proof shows that if $\alpha < 0$ and $\underline{\mu} \geq 0$ then $m = -\infty$ for all $q \in (2, 2^\star]$. The choice of q was needed only in the other region.

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Table of Notation

Notation applies to any $s \in \mathbb{R}$, $\nu \geq 0$, $(\alpha, \beta) \in \mathbb{R}^2$, $j, k \in \mathbb{Z}$, $Z \in \mathbb{R}^3$, $I \subset \mathbb{R}$, $\varphi, \psi \in H^1(\mathbb{R}^d)$, $u \in C_t(H^1_x(\mathbb{R}^d))$, any suffix $\diamondsuit, \heartsuit$, any sequence $\varphi_n \in H^1(\mathbb{R}^d)$, and any functional G on $H^1(\mathbb{R}^d)$.

Dimension and scaling	$d \in \mathbb{N}$, $2_\star, 2^\star > 0$: space dimension and critical powers	(1-3)
	$\alpha, \beta \in \mathbb{R}$, $\bar{\mu} \geq \underline{\mu} \geq 0$: scaling exponents and their functions	(2-1)
	$\varphi^\lambda_{\alpha,\beta}$, $\mathscr{L}_{\alpha,\beta} G$: rescaled family and scaling derivative	(1-13) (1-14)
	(subscript $\diamondsuit_{\alpha,\beta}$ and $\heartsuit_{\alpha,\beta}$ are often written as $\diamondsuit$ and $\heartsuit$)	
1st order representation	$\vec{u} \leftrightarrow u$: linked with each other by	(4-1)
Nonlinearity	$F(\varphi)$, $f(s) \geq 0$: nonlinear energy and its density	(1-11)
	$f_S(s)$, $f_L(s) \geq 0$: small and large parts of f	(1-24)
	$p_1, p_2 > 0$, $\kappa_0 \geq 0$: leading powers of f_S and f_L	(1-25) (1-26) (1-29)
Functionals	$J(\varphi), J^{(\nu)}(\varphi) \in \mathbb{R}$: static energy, with mass change	(1-11) (1-12)
	$K_{\alpha,\beta}(\varphi)$, $K^{(c)}_{\alpha,\beta}(\varphi) \in \mathbb{R}$, $H_{\alpha,\beta}(\varphi) \geq 0$: derivatives of J	(1-15) (2-26)
	$K^Q_{\alpha,\beta}(\varphi)$, $K^N_{\alpha,\beta}(\varphi) \in \mathbb{R}$: quadratic and nonlinear parts of K	(2-2)
	$E(u;t), E(\varphi,\psi), e(u) \in \mathbb{R}$: total energy and its density	(1-5) (7-14)
	$E^Q(u;t)$, $E^Q(\varphi,\psi) \geq 0$: linear energy	(1-37)
	$\widetilde{E}(\varphi)$, $\widetilde{K}_{\alpha,\beta}(\varphi) \in \mathbb{R}$: vector versions of E and K	(4-3)
	$P(u;t), E_{R,c}(u;t) \in \mathbb{R}$: momentum and exterior energy	(7-7) (7-5)
	$X_R(u;t), V_R(u;t) \in \mathbb{R}$: localized energy center and virial	(7-13) (7-25)
Variational splittings	$m_{\alpha,\beta}$, $E^\star \geq 0$: static and scattering energy thresholds	(1-17) (6-1)
	$\mathscr{K}^\pm_{\alpha,\beta}$, $\widetilde{\mathscr{K}}^+_{\alpha,\beta}$: splitting below the threshold	(1-18) (4-5)
	$C^\nu_{\mathrm{TM}}(G), C^\star_{\mathrm{TM}}(G) \in [0,\infty]$: Trudinger–Moser ratio	(2-47) (2-49)
	$\mathfrak{M}(G) \in [0,\infty]$: Trudinger–Moser threshold on $\dot{H}^1$	(2-48)
	$\operatorname{conc} G((\varphi_n)_n) \in \mathbb{R}$: concentration at $x = 0$	(2-51)
Function spaces and exponents	$[Z]_\nu(I), [Z]_0(I), [Z]^\bullet_\nu(I)$: Lebesgue–Besov spaces on $I \times \mathbb{R}^d$	(4-7)
	$Z^s, Z^{*(s)} \in \mathbb{R}^3$: regularity change and dual of exponents	(4-9)
	$\operatorname{reg}^\theta(Z), \operatorname{str}^\theta(Z), \operatorname{dec}^\theta(Z) \in \mathbb{R}$: regularity and decay indexes	(4-8)
	$H, W, K, M^\sharp, V \in \mathbb{R}^3$: exponents for $d \in \mathbb{N}$	(4-24) (4-31) (5-68)
	$X, S, L \in \mathbb{R}^3$: exponents for $d \leq 4$	(4-31) (4-54)
	$\widetilde{M}, M, \widehat{M}, \widetilde{N}, N, Q, P, Y, R, G \in \mathbb{R}^3$: exponents for $d \geq 5$	(4-68) (4-69) (5-87)
	$H_\varepsilon, W_\varepsilon, M^\sharp_\varepsilon \in \mathbb{R}^3$: exponents for $d \geq 5$	(5-81)
	H^1_ν, $\mathcal{MC}$: $H^1(\mathbb{R}^2)$ and a set of Fourier multipliers on $\mathbb{R}^d$	(4-38) (5-2)
	$\mathscr{X}$, $\mathscr{Y}$, $\mathscr{Y}_0$, $\widetilde{\mathscr{Y}}$, $\mathscr{Y}^*_0$, $\mathscr{Y}^*$: Strichartz-type spaces	(4-54) (4-77)
	$ST(I), ST^*(I), ST^\diamondsuit_\infty(I)$: Strichartz-type spaces on $I \times \mathbb{R}^d$	(5-59) (5-60)
Profile decomposition	$(t^\diamondsuit_\heartsuit, x^\diamondsuit_\heartsuit, h^\diamondsuit_\heartsuit) \in \mathbb{R}^{1+d} \times [0,1]$: time-space-scale shift parameter	page 438
	$\gamma^\diamondsuit_\heartsuit = -t^\diamondsuit_\heartsuit / h^\diamondsuit_\heartsuit \in \mathbb{R}$: rescaled time shift	
	$h^\diamondsuit_\infty \in \{0,1\}, \gamma^\diamondsuit_\infty \in [-\infty,\infty]$: limit of $h^\diamondsuit_n$ and $\gamma^\diamondsuit_n$	
	$T^\diamondsuit_\heartsuit \varphi$, $\langle\nabla\rangle_\heartsuit \diamondsuit \varphi$: operators dependent on $(x^\diamondsuit_\heartsuit, h^\diamondsuit_\heartsuit)$	(5-1)
	$(t^{jl}_n, x^{jl}_n, h^{jl}_n)$, $S^{jl}_n u$: relative shift and transform	(5-21) (5-20)
	$\tau^\diamondsuit_\heartsuit \in \mathbb{R}$, $\tau^\diamondsuit_\infty \in [-\infty,\infty]$: scaled time shift and its limit	(5-1)
	$\vec{U}^\diamondsuit_\infty$, $\widehat{U}^\diamondsuit_\infty$, : nonlinear profiles (scaled limit)	(5-52) (5-53)
	$\vec{u}^j_{(n)}$, $\vec{u}^{<k}_{(n)}$: nonlinear profiles (in original scales)	(5-54) (5-58)

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RAYLEIGH-TYPE SURFACE QUASIMODES IN GENERAL LINEAR ELASTICITY

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Rayleigh-type surface waves correspond to the characteristic variety, in the elliptic boundary region, of the displacement-to-traction map. In this paper, surface quasimodes are constructed for the reduced elastic wave equation, anisotropic in general, with traction-free boundary. Assuming a global variant of a condition of Barnett and Lothe, the construction is reduced to an eigenvalue problem for a selfadjoint scalar first order pseudodifferential operator on the boundary. The principal and the subprincipal symbol of this operator are computed. The formula for the subprincipal symbol seems to be new even in the isotropic case.

1. Introduction

Rayleigh [1887] discovered the existence of surface waves which propagate along a traction-free flat boundary of an isotropic elastic body and which decay exponentially into the interior. The propagation speed of the surface wave is strictly less than that of body waves. Barnett and Lothe [1976] showed that Rayleigh-type surface waves can also exist at flat boundaries of anisotropic elastic media.

The goal of this paper is to construct, for elastic media which are not necessarily isotropic, Rayleigh-type surface quasimodes which are asymptotic to eigenvalues or resonances. We use a geometric version of semiclassical microlocal analysis.

The Rayleigh wave phenomenon of isotropic elastodynamics was explained by Taylor [1979] as propagation of singularities, over the elliptic boundary region, for the Neumann (displacement-to-traction) operator. Nakamura [1991] generalized this to anisotropic media, using the theory of Barnett and Lothe. Assuming isotropy of the elastic medium, Cardoso and Popov [1992] and Stefanov [2000] constructed Rayleigh quasimodes.

Let (M, g) be an oriented Riemannian manifold with nonempty compact smooth boundary X. The (infinitesimal) displacement of an elastic medium occupying M is a vector field u on M. The Lie derivative of the metric tensor is a symmetric tensor field, $\operatorname{Def} u = \mathcal{L}_u g/2$, called the deformation (strain) tensor caused by the displacement u. The elastic properties are defined by the elasticity (stiffness) tensor. This is a real fourth order tensor field $C \in C^\infty(M; \operatorname{End}(T^{0,2}M))$, $e \mapsto Ce$, which maps into symmetric tensors and vanishes on antisymmetric tensors. We assume positive definiteness of C, i.e., $(e \mid f)_C = (Ce \mid f)$ defines an inner product on the space of symmetric tensors e and f. Here $(\cdot|\cdot)$ denotes the inner product on tensors induced from g. This assumption is often called the strong convexity condition. If coordinates are given, then the components of C satisfy symmetries, $C^{ijk\ell} = C^{jik\ell} = C^{k\ell ij}$, and $C^{ijk\ell} e_{ij} e_{k\ell} > 0$ if e_{ij} is a nonzero symmetric tensor. (We use the summation convention.) Denote the

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Riemannian volume elements on M and X by $\mathrm{d}V_M$ and $\mathrm{d}V_X$, respectively. The elasticity operator L and the traction T are defined, on compactly supported vector fields, by

$$\int_M (\operatorname{Def} u \mid \operatorname{Def} v)_C \, \mathrm{d}V_M = \int_M (Lu \mid v)\, \mathrm{d}V_M + \int_X (Tu \mid v)\, \mathrm{d}V_X. \tag{1}$$

A positive mass density $\rho \in C^\infty(M)$ and the elasticity tensor C define the material properties of the elastic medium. If the surface X is traction-free, then vibrations of the medium are solutions of the following eigenvalue problem: $Lu = \lambda^2 \rho u$ in M, $Tu = 0$ at X. See [Marsden and Hughes 1983] for linear elasticity in the language of Riemannian geometry.

The principal symbol of L, and of the h-differential operator $h^2 L$, equals the acoustic tensor, $c(\xi) = c(\xi, \xi) \in \operatorname{End}(\mathbb{C}T_x M)$, $\xi \in T_x^* M$; see (31). Here the associated acoustical tensor $c(\xi, \eta) \in \operatorname{End}(\mathbb{C}T_x M)$, $\xi, \eta \in T_x^* M$, is defined as follows:

$$\big(c(\xi,\eta) v \mid w\big) = \big(v \otimes \eta \mid w \otimes \xi\big)_C. \tag{2}$$

(Using g, we identify vectors with covectors.) The ik-th covariant component of $c(\xi,\eta)$ equals $C^{ijk\ell}\xi_j \eta_\ell$.

The existence of Rayleigh waves depends on the characteristic variety, Σ, of the surface impedance tensor, z. To define z, we first recall the definition of the elliptic boundary region, $\mathscr{E} \subset T^*X$. Let ν denote the unit exterior conormal field of the boundary X. Identify $T^*X = \nu^\perp \subset T_X^* M$. By definition, $\xi \in \mathscr{E}$ if and only if $c(\xi + s\nu) - \rho \operatorname{Id}$ is positive definite for real s. From the factorization theory of selfadjoint matrix polynomials one gets $q(\xi) \in \operatorname{End}(\mathbb{C}T_x M)$, $\xi \in \mathscr{E} \cap T_x^* X$, such that

$$c(\xi + s\nu) - \rho \operatorname{Id} = \big(s \operatorname{Id} - q^*(\xi)\big) c(\nu) \big(s \operatorname{Id} - q(\xi)\big), \tag{3}$$

$s \in \mathbb{C}$. Moreover, the spectrum of $q(\xi)$ lies in the lower half-plane, $\operatorname{spec} q(\xi) \subset \mathbb{C}_-$, and these properties determine $q(\xi)$ uniquely. The surface impedance tensor z is defined as follows:

$$z(\xi) = i c(\nu) q(\xi) + i c(\nu, \xi), \quad \xi \in \mathscr{E}. \tag{4}$$

The significance of z results from the fact, proved in Lemma 18, that z is the principal symbol of a parametrix of the displacement-to-traction operator. In physics, the meaning of z is that it relates the amplitudes of displacements to the amplitudes of tractions (forces) needed to sustain these.

The surface impedance tensor is Hermitian, and positive definite for large $|\xi|$ [Barnett and Lothe 1985, Theorem 6]. If $\dim M = 3$, then

$$z(\xi),\ \xi \in \mathscr{E}, \text{ has at most one nonpositive eigenvalue.} \tag{U}$$

This property expresses the uniqueness of Rayleigh-type surface waves [Barnett and Lothe 1985, Theorem 8]. In case $\dim X \neq 3$, we shall assume (U) as a hypothesis. The characteristic variety of z,

$$\Sigma = \{\xi \in \mathscr{E}\,;\, \det z(\xi) = 0\},$$

is a smooth hypersurface, transversal to the radial directions of the fibers of T^*X. Compare [Barnett and Lothe 1985, Theorem 7]. Rayleigh waves exist only if Σ is not empty. We shall make the stronger assumption that Σ intersects every radial line:

$$\Sigma \cap \mathbb{R}_+ \xi \neq \varnothing \quad \text{if } \xi \in T^*X \setminus 0. \tag{E1}$$

Compare [Barnett and Lothe 1985, Theorem 12], [Nakamura 1991, Theorem 2.2], [Kawashita and Nakamura 2000, (ERW)]. Assuming (U) and (E1), there exists a unique $p \in C^\infty(T^*X \setminus 0)$, $p > 0$, homogeneous of degree 1, such that

$$\Sigma = p^{-1}(1). \tag{5}$$

See Proposition 6. Furthermore, the kernel of z defines a line bundle, $\ker z \to \Sigma$, over the compact base Σ. We shall require that its first Chern class vanishes:

$$\ker z \to \Sigma \text{ is a trivial line bundle.} \tag{E2}$$

In particular, the bundle is assumed to possess a unit section. Property (E2) is stable with respect to homotopies in the material properties; see Corollary 7. In the case of isotropic elasticity with positive Lamé parameters, (U), (E1), and (E2) hold. Moreover,

$$\Sigma = \{c_r|\xi| = 1\} \subset \mathscr{E} = \{c_s|\xi| > 1\}, \quad p(\xi) = c_r|\xi|.$$

Here c_r is the propagation speed of the Rayleigh surface wave which is strictly less than the speeds of the body waves, $0 < c_r < c_s < c_p$. See Example 8.

Next we state the central result of this paper: The traction-free surface eigenvalue problem can be intertwined with a selfadjoint eigenvalue problem on the boundary. We employ a semiclassical pseudo-differential calculus, with distributions and operators depending on a small parameter, $0 < h \leq 1$. We write $A_h \equiv B_h$ if and only if the Schwartz kernel of $A_h - B_h$ belongs to C^∞ with seminorms satisfying $\mathbb{O}_{C^\infty}(h^\infty)$.

Theorem 1. *Assume* $\dim M = 3$, *or* (U). *Assume* (E1), (E2). *Given a unit section v of* $\ker z \to \Sigma$, *there exists a selfadjoint, elliptic operator $P \in \Psi^1(X; \Omega^{1/2})$, independent of h, and operators,*

$$B_h : L^2(X; \mathbb{C}T_X M) \to L^2(M; \mathbb{C}TM), \quad \|B_h\| = \mathbb{O}(h^{1/2}),$$
$$J_h, \tilde{J}_h \in \Psi^{0,0}(X; \Omega^{1/2}, \mathbb{C}T_X M), \quad J_h^* J_h \text{ elliptic at } \Sigma,$$

such that

$$\big(h^2 L - \rho\big) B_h \equiv 0, \quad T B_h J_h \equiv \tilde{J}_h (P - h^{-1}),$$

and $B_h|_X = \mathrm{Id}$ in a neighborhood of Σ. The principal symbol of P equals p of (5). *Furthermore, there is a formula,* (50), *for the subprincipal symbol p_{sub} of P. If v is changed to another unit section, $e^{i\varphi} v$, then the subprincipal symbol changes to $p_{\mathrm{sub}} + \{p, \varphi\}$, where $\{p, \varphi\}$ denotes the Poisson bracket.*

This result is known in the isotropic case [Cardoso and Popov 1992; Stefanov 2000], except for the assertions about the subprincipal symbol.

The operator B_h is a parametrix of the Dirichlet problem near Σ; see Proposition 17. Its range consists of functions which are smooth in the interior of M, supported in a preassigned neighborhood of the boundary, and which decay like $e^{-\delta \operatorname{dist}_X / h}$ into the interior.

Ignoring finitely many eigenvalues the spectrum of P consists of a sequence of positive eigenvalues $\mu_j \uparrow \infty$. Applying Theorem 1 to an associated orthonormal system of eigenvectors we obtain, in Proposition 21, a sequence of quasimode states: $L u_j - \mu_j^2 \rho u_j = \mathbb{O}_{C^\infty}(h_j^\infty)$ with boundary tractions equal to zero. Moreover, the quasimode states are well-separated. The construction also works when starting with a sequence of almost orthogonal quasimode states of P.

Let $D = \{u \in C_c^\infty\,;\, Tu = 0\}$. The unbounded operator $D \to L^2(M; \mathbb{C}TM; \rho\,\mathrm{d}V_M)$, $u \mapsto \rho^{-1}Lu$, is symmetric and nonnegative. The associated quadratic form is given by the left-hand side of (1). Denote by L_T the Friedrichs extension of this operator. For a selfadjoint operator A with spectrum consisting of a sequence of eigenvalues accumulating at $+\infty$, denote by $N_A(\lambda)$ the usual counting function for the eigenvalues of A. The following lower bound on $N_{L_T}(\lambda)$ is an example application of our results.

Corollary 2. *Assume M compact*, $\dim M = 3$, *and* (E1), (E2). *Let P be the selfadjoint operator given in Theorem 1. For every $m > 1$, $N_{L_T}(\lambda) - N_P(\lambda - \lambda^{-m})$ is bounded from below.*

Rayleigh waves have been studied in several papers with the emphasis of getting information about resonances in scattering theory [Stefanov and Vodev 1994; 1995; 1996; Sjöstrand and Vodev 1997; Vodev 1997; Stefanov 2000], and, for anisotropic media, [Kawashita and Nakamura 2000]. Stefanov [2000] uses Rayleigh quasimodes to derive lower bounds on the number of resonances. See the remark at the end of Section 9 about going from quasimodes to resonances.

The subprincipal symbol p_{sub} affects the eigenvalue asymptotics of P [Duistermaat and Guillemin 1975], and it enters quasimode constructions [Cardoso and Popov 1992]. The subprincipal symbol occurs in the final formulas via integrals, such as $\int_{S^*X} p_{\mathrm{sub}}$ and $\int_\gamma p_{\mathrm{sub}}$, where γ is a closed bicharacteristic. We point out that these integrals do not depend on the choice of the unit section v in Theorem 1, although p_{sub} itself does. An important aim of the present work is to give explicit formulas for the subprincipal symbol of P. These seem to be new even in the isotropic case which is dealt with in more detail in Proposition 25. The main difficulty comes from the fact that an invariant notion of subprincipal symbol has only been available for scalar operators. To overcome this obstacle we adapt and systematically use the geometric pseudodifferential calculus of Sharafutdinov [2004; 2005] which assumes given a differential geometric structure. The principal and subprincipal symbol levels are contained in the leading symbol of a (pseudo-)differential operator.

The paper is organized as follows. In Section 2 the surface impedance tensor is studied; in particular, a selfcontained treatment of Barnett–Lothe theory is given. The leading geometric symbols of some differential operators are computed in Section 3. In Section 4 we geometrically decompose the elasticity operator near the boundary into normal and tangential operators, keeping track of leading geometric symbols. Section 5 gives, microlocally at the elliptic region $\mathscr{E}$, a factorization of $h^2L - \rho$ into a product of first order operators. Using the factorization, we construct in Section 6 a parametrix for the Dirichlet problem microlocally at $\mathscr{E}$. The displacement-to-traction operator Z is defined in Section 7, and its leading geometric symbol is determined. In Section 8 we derive a diagonalization of Z, and we prove Theorem 1. In Section 9 we construct localized traction-free surface quasimodes, and we prove Corollary 2. In Section 10 we calculate, for an isotropic elastic medium, the subprincipal symbol of P. The Appendix contains a detailed exposition of Sharafutdinov's geometric pseudodifferential calculus in a semiclassical setting.

2. The surface impedance tensor

First we collect some well-known facts about spectral factorizations of selfadjoint matrix polynomials. Refer to [Gohberg et al. 1982, Chapter 11]. Let V be a finite-dimensional complex Hilbert space, and $f(s) = as^2 + bs + c \in \mathrm{End}(V)$ a quadratic polynomial in the complex variable s. The spectrum of f is the set of $s \in \mathbb{C}$ such that $\ker f(s) \neq 0$. Assume that the leading coefficient of f, a, is nonsingular. Then the spectrum is finite. Assume that f is selfadjoint, $f(s)^* = f(\bar{s})$, and that, in addition $f(s)$ is positive definite for real s. The spectrum of f is a disjoint union $\sigma_+ \cup \sigma_-$, where σ_+ and σ_- are contained in the upper and lower half-planes, respectively. There is a unique $q \in \mathrm{End}(V)$ such that $f(s) = (s-q^*)a(s-q)$, and the spectrum of q equals σ_-. If γ is a closed Jordan curve which contains σ_- in its interior and σ_+ in its exterior, then

$$q \oint_\gamma f(s)^{-1} \mathrm{d}s = \oint_\gamma s f(s)^{-1} \mathrm{d}s. \tag{6}$$

The integral on the left is nonsingular. Jordan–Keldysh chains are a means to compute q. In particular, one has $qv = sv$ if $f(s)v = 0$ and $\operatorname{Im} s < 0$. Moreover, the solvency equation $f(q) = 0$ holds.

The following representation of the factor q by integrals is important. We shall also apply it later to establish symbol properties. Denote by $i = \sqrt{-1}$ the imaginary unit.

Lemma 3. *Let f and q be as above. Then*

$$a\, q f_0 = -\pi i \,\mathrm{Id} + f_1, \tag{7}$$

where $f_0 = \int_{-\infty}^{\infty} f(s)^{-1} \mathrm{d}s$ is selfadjoint and positive definite, and

$$f_1 = \int_{|s|\le 1} s a f(s)^{-1} \mathrm{d}s + \int_{|s|>1} s^{-1}\big(s^2 a - f(s)\big) f(s)^{-1} \mathrm{d}s.$$

The integrals converge absolutely in $\mathrm{End}(V)$.

Proof. Let γ_R be the negatively oriented closed contour composed of the semicircle $\{|s| = R, \operatorname{Im} s \le 0\}$ and the interval $[-R, R]$. The integral representation (6) holds with $\gamma = \gamma_R$ if R is sufficiently large. We have $f(s)^{-1} = s^{-2}a^{-1} + \mathbb{O}(|s|^{-3})$ as $|s| \to \infty$. It follows that

$$\lim_{R\to\infty} \oint_{\gamma_R} f(s)^{-1} \mathrm{d}s = \int_{-\infty}^{\infty} f(s)^{-1} \mathrm{d}s$$

and

$$\lim_{R\to\infty} \oint_{\gamma_R} s a f(s)^{-1} \mathrm{d}s = -\pi i \,\mathrm{Id} + \lim_{R\to\infty} \int_{-R}^{R} s a f(s)^{-1} \mathrm{d}s.$$

Using $s^2 a f(s)^{-1} - \mathrm{Id} = (s^2 a - f(s)) f(s)^{-1}$ we obtain

$$\int_{1<|s|\le R} s a f(s)^{-1} \mathrm{d}s = \int_{1<|s|\le R} s^{-1}\big(s^2 a - f(s)\big) f(s)^{-1} \mathrm{d}s.$$

This proves the formulas. The remaining assertions follow from these and the positive definiteness of $f(s)$. □

Let $\xi \in T_x^* X$, and denote by $\nu \in T_x^* M$ the unit exterior normal. Set $a = c(\nu)$, $a_1(\xi) = c(\nu, \xi)$, and $a_2(\xi) = c(\xi)$. Note that $a_1(\xi)^* = c(\xi, \nu)$. The polynomial

$$f(s) = c(\xi + s\nu) - \rho = a s^2 + (a_1 + a_1^*) s + a_2 - \rho, \tag{8}$$

$f(s) = f(s, \xi)$, has values in $\mathrm{End}(\mathbb{C} T_x M)$. It is selfadjoint with real coefficients. By definition, $\xi \in \mathscr{E}$ if and only if $f(s)$ is positive definite for $s \in \mathbb{R}$.

Lemma 4. *The elliptic region $\mathscr{E}$ is an open subset of $T^* X$ with compact complement. Moreover, $\mathscr{E}$ is symmetric and star shaped with respect to infinity, i.e., $t\xi \in \mathscr{E}$ whenever $\xi \in \mathscr{E}$ and t real, $|t| \ge 1$.*

Proof. By positive definiteness of C, there exists $\delta > 0$ such that $g(v, c(\eta)v) \geq \delta|v \otimes \eta + \eta \otimes v|^2$ for (co-)vectors v, η. The symmetrization of a nonzero real elementary tensor is nonzero. Therefore, with a new $\delta > 0$, in the sense of selfadjoint maps,

$$c(\eta) \geq \delta|\eta|^2 \,\mathrm{Id}\,. \tag{9}$$

Since $|\xi + sv|^2 = |\xi|^2 + s^2$ the first assertions follow. The symmetry and the star-shapedness follow from $c(t\eta) = t^2 c(\eta)$. □

If $\xi \in \mathscr{E}$, then (7) holds with $q = q(\xi)$, $f_j = f_j(\xi)$. The spectral factor q solves (3); using current notation:

$$as^2 + (a_1 + a_1^*)s + a_2 - \rho = (s - q^*)a(s - q). \tag{10}$$

The spectrum of q lies in the lower half-plane, and q is uniquely determined by these properties. Notice that q is a smooth section of the bundle $\pi^* \operatorname{End}(\mathbb{C}T_X M) \to \mathscr{E}$, where $\pi : \mathscr{E} \subset T^*X \to X$ denotes the canonical projection.

The surface impedance tensor, defined in (4), equals $z = i(aq + a_1)$. Lemma 3 implies

$$zf_0 = \pi \,\mathrm{Id} + i(f_1 + a_1 f_0). \tag{11}$$

Since the f_j's are real, this gives the decomposition of z into real and imaginary parts. Following [Mielke and Fu 2004], we shall use the Riccati-type equation

$$(z + ia_1^*)a^{-1}(z - ia_1) = a_2 - \rho \tag{12}$$

to deduce properties of z. Equation (12) follows upon insertion of $q = -a^{-1}(iz + a_1)$ into the solvency equation associated with (10),

$$aq^2 + (a_1 + a_1^*)q + a_2 - \rho = 0. \tag{13}$$

A consequence of (12) is

$$(iq)^* z' + z'(iq) = a_1^{*\prime} q + q^* a_1' + (a_2 - \rho)' + q^* a' q, \tag{14}$$

where the prime denotes the derivative with respect to some chosen parameter. The spectra of q and q^* are disjoint. Therefore, the Sylvester equation $(iq)^*x + x(iq) = i(xq - q^*x) = y$ has a unique solution x for given y. The solution is, in fact, given by an integral, $x = \int_{-\infty}^0 \exp(irq)^* y \exp(irq)\,\mathrm{d}r$. It follows that x is positive definite if y is.

Proposition 5. *The impedance tensor $z(\xi)$, $\xi \in \mathscr{E}$, has the following properties.*

(i) $z(\xi)$ *is selfadjoint.*

(ii) $z(\xi)$ *is positive definite if* $|\xi|$ *is sufficiently large.*

(iii) $\operatorname{Re} z(\xi)$ *is positive definite.*

(iv) $z(\xi)$ *has at least two positive eigenvalues if* $\dim M \geq 3$.

(v) $(d/dt)|_{t=1} t^{-1} z(t\xi) = \dot{z} - z$ *is positive definite.*

(vi) *The complex conjugate* $\overline{z(\xi)} = z(-\xi)$.

We call $\dot{z}(\xi) = (d/dt)|_{t=1} z(t\xi)$ the radial derivative of z at ξ. It follows from (v) that $\dot{z}$ is positive definite on the kernel of z, $\ker z$.

Proof. To prove (i) we follow the arguments in [Mielke and Fu 2004, Theorem 2.2]. First note that (12) remains true if z is replaced by z^*. Subtracting the two equations we get the Sylvester equation $(iq)^*(z-z^*)+(z-z^*)(iq)=0$, implying $z-z^*=0$.

It follows from (11) that $\operatorname{Re} z=\pi f_0^{-1}$. This proves (iii).

Suppose $\dim M\geq 3$. Aiming at an indirect proof of (iv), assume that $z(\xi)$, $\xi\in T_x^*X$, has at most one positive eigenvalue. Then there exists $w\in\mathbb{C}T_xM$ such that $z(\xi)$ is negative semidefinite on the orthogonal complement $w^\perp$. Choose a real vector $v\neq 0$ which is orthogonal to both $\operatorname{Re} w$ and $\operatorname{Im} w$. Then $v\in w^\perp$, and $(\operatorname{Re} z(\xi)v\mid v)=(z(\xi)v\mid v)\leq 0$, contradicting the positive definiteness of $\operatorname{Re} z$.

Next we prove (v) following the method of [Mielke and Fu 2004, Theorem 2.3]. Since $a_j(\xi)$ is homogeneous of degree j in ξ, (12) implies

$$(t^{-1}z(t\xi)+ia_1^*(\xi))a^{-1}(t^{-1}z(t\xi)-ia_1(\xi))=a_2(\xi)-t^{-2}\rho.$$

Taking the derivative with respect to t at $t=1$, we get

$$(iq)^*(\dot z-z)+(\dot z-z)(iq)=2\rho.$$

By the remarks following (14), we see that $\dot z-z$ is positive definite.

We now prove (vi). Note $\overline{f(s,-\xi)}=f(-s,\xi)$, $f_j(-\xi)=(-1)^j f_j(\xi)$, and $a_1(-\xi)=-a_1(\xi)$. Using (11) we derive $z(-\xi)f_0(\xi)=\overline{z(\xi)f_0(\xi)}$. Since f_0 is real and nonsingular the formula follows.

It remains to prove (ii). Let $\eta\in T_xX$, $|\eta|=1$. It suffices to show that $z_\infty=\lim_{t\uparrow\infty}t^{-1}z(t\eta)$ exists and is positive definite. Set $q_t=t^{-1}q(t\eta)$, $t>1$ large. From (10) deduce

$$as^2+(a_1(\eta)+a_1^*(\eta))s+a_2(\eta)-t^{-2}\rho=(s-q_t^*)a(s-q_t),\quad s\in\mathbb{R}.$$

Using (7) and dominated convergence in the integrals giving f_j we infer that $q_\infty=\lim_{t\uparrow\infty}q_t$ exists. In particular, $t^{-1}z(t\eta)$ converges to $z_\infty=i(aq_\infty+a_1(\eta))$ as $t\uparrow\infty$. Let $y\in T_xM$ such that $(z_\infty y\mid y)\leq 0$. We must show $y=0$. Set $w(r)=\exp(irq_\infty)y$, $r\leq 0$. The solvency Equation (13) holds with q replaced by q_∞, $\rho=0$. Therefore, $aD_r^2w+(a_1+a_1^*)D_rw+a_2w=0$ holds, where we use the abbreviation $a_j=a_j(\eta)$. Take the inner product in $\mathbb{C}T_xM$ with w and integrate. An integration by parts gives

$$\int_{-\infty}^0(aD_rw+a_1w\mid D_rw)+(D_rw\mid a_1w)+(a_2w\mid w)\,\mathrm{d}r=i(aD_rw+a_1w\mid w)\big|_{-\infty}^0=(z_\infty y\mid y)\leq 0.$$

Set $W(r)=w(r)\otimes\eta+D_rw(r)\otimes\nu\in\operatorname{End}(\mathbb{C}T_xM)$. Recall $a=c(\nu)$, $a_1=c(\nu,\eta)$, $a_2=c(\eta)$, and (2). We have shown:

$$\int_{-\infty}^0(W(r)\mid W(r))_C\,\mathrm{d}r\leq 0.$$

Recall that C is real, and that $(\cdot\mid\cdot)_C$ is an inner product on symmetric 2-tensors. It follows that the symmetrization of $W(r)$ vanishes for all $r\leq 0$. In particular,

$$\big(w(r)\otimes\eta+D_rw(r)\otimes\nu\mid\zeta\otimes\nu+\nu\otimes\zeta\big)=0\tag{15}$$

for $\zeta\in\mathbb{C}T_x^*M$, $r\leq 0$. Recall $(\eta\mid\nu)=0$. Setting $\zeta=\nu$, we derive $D_r(w(r)\mid\nu)=(D_rw(r)\mid\nu)=0$. Since $w(r)\to 0$ as $r\to-\infty$, we obtain $(w(r)\mid\nu)=0$. Now, (15) simplifies to $(D_rw(r)\mid\zeta)=0$. Since ζ is arbitrary, this implies, successively, $D_rw=0$, $w=0$, $y=0$. ☐

If $\dim M = 3$ then (U) holds. This follows from (iv).

Proposition 6. *Assume* (U). *Then the characteristic variety of* z, $\Sigma = \{\det z(\xi) = 0\}$, *is a smooth hypersurface in* $\mathscr{E}$. *Each radial line* $\mathbb{R}_+\xi \subset T^*X$ *intersects* Σ *in at most one point, and the intersection is transversal. The kernel of* $z|_\Sigma$ *defines a line bundle* $\ker z \to \Sigma$. *Assume, in addition,* (E1). *There is a unique* $p \in C^\infty(T^*X \setminus 0)$, *homogeneous of degree one, such that* $\Sigma = p^{-1}(1)$. *Moreover,* $p > 0$, *and* $p(-\xi) = p(\xi)$.

Proof. From the assumption and (v) of Proposition 5 it follows that $(d/dt)\det z(t\xi) > 0$ if $t\xi \in \Sigma$, $t > 0$. In particular, zero is a regular value of $\det z$. Hence Σ is a codimension one submanifold transversal to the radial field. Since $\mathbb{R}_+\xi \cap \mathscr{E}$ is connected, a given radial line $\mathbb{R}_+\xi$ intersects Σ in at most one point. Because of (U) and the selfadjointness of z, zero is simple eigenvalue of z. It follows that $\ker z \to \Sigma$ is a line bundle. Now assume also (E1). Then each radial line intersects Σ in a unique point. Define p as follows. For $0 \neq \xi \in T^*X$ set $p(\xi) = 1/t$ if $t\xi \in \Sigma$, $t > 0$. Smoothness of p follows from the implicit function theorem. The evenness of p is a consequence of (vi). The other properties of p are obvious. Clearly, the homogeneity and $p|_\Sigma = 1$ determine p uniquely. □

Corollary 7. *Let* ρ_t *and* C_t *be homotopies of the mass densities and the elasticity tensors,* $0 \leq t \leq 1$. *Assume that the associated surface impedance tensors* z_t *and their characteristic varieties* Σ_t *satisfy* (U) *and* (E1) *for every* t. *The line bundles* $\ker z_0 \to \Sigma_0$ *and* $\ker z_1 \to \Sigma_1$ *are isomorphic.*

Proof. The factorization (3) and the definition of the impedance tensor imply that z_t depends continuously on the homotopy parameter t. It follows from Proposition 6 that the characteristic varieties are canonically diffeomorphic to the sphere bundle SX. We deduce that the Chern classes of the bundles $\ker z_t \to SX$ do not depend on t. The assertion follows from this. □

Example 8. We consider, as special case, an isotropic elastic medium. We shall verify (U), (E1), and (E2). The elasticity tensor reads, in component notation,

$$C^{ijk\ell} = \lambda g^{ij} g^{k\ell} + \mu(g^{ik} g^{j\ell} + g^{i\ell} g^{jk}), \tag{16}$$

where λ, μ denote the Lamé parameters. Equivalently,

$$c(\xi, \eta) = \lambda\xi \otimes \eta + \mu\eta \otimes \xi + \mu g(\xi, \eta)\,\mathrm{Id}. \tag{17}$$

Positive definiteness of C is equivalent to $\mu > 0$, $\lambda \dim M + 2\mu > 0$. We make the stronger assumption $\lambda, \mu > 0$. Let $\xi \in T^*_x X$. We list the eigenvalues $s \in \mathbb{C}$ and the eigenvectors $v \in \mathbb{C}T_x M$ of the quadratic polynomial $c(\xi + s\nu) - \rho$:

(a) $(\lambda + 2\mu)(|\xi|^2 + s^2) - \rho = 0$ and $v = \xi + s\nu$,

(b) $\mu(|\xi|^2 + s^2) - \rho = 0$ and $v = s\xi - |\xi|^2\nu$,

(c) $\mu(|\xi|^2 + s^2) - \rho = 0$ and v is orthogonal to ξ and ν.

Introduce $c_p = \sqrt{(\lambda + 2\mu)/\rho}$ and $c_s = \sqrt{\mu/\rho}$, the speeds of pressure and of shear waves, respectively. Assume that $\xi \in \mathscr{E}$. This is equivalent to $c_s|\xi| > 1$. The above eigenvalues and eigenvectors diagonalize q, $q(\xi)v = sv$ if $\operatorname{Im} s < 0$. Denote by V the subbundle of $\pi^*\big(\mathbb{C}T_X M\big) \to \mathscr{E}$ spanned by ν and ξ, and $V^\perp$ its orthogonal bundle. Fix the orthonormal frame $\nu, \hat{\xi} = \xi/|\xi|$ of V, and choose an orthonormal frame of $V^\perp$. In block decompositions of matrices we let the indices 1 and 2 correspond to V and

$V^\perp$, respectively. We denote by $(e)_{ij}$ the block ij of the matrix which represents the endomorphism e. Observe that q leaves V and $V^\perp$ invariant, $(q)_{12} = 0 = (q)_{21}$. A simple computation gives

$$(iq)_{11} = \frac{|\xi|}{b} \begin{bmatrix} ut\sqrt{1-t} & -i(b-ut) \\ i(b-t) & t\sqrt{1-ut} \end{bmatrix}. \tag{18}$$

Here $t = (c_s|\xi|)^{-2}$, $u = (c_s/c_p)^2 = \mu/(\lambda+2\mu)$, $b = 1-\sqrt{1-ut}\sqrt{1-t}$. Moreover, $(iq)_{22}$ equals $|\xi|\sqrt{1-t}$ times the unit matrix. The maps $a = c(\nu)$ and $a_1 = c(\nu,\xi)$ also leave V and $V^\perp$ invariant. We compute

$$(z)_{11} = \frac{\mu|\xi|}{b} \begin{bmatrix} t\sqrt{1-t} & -i(2b-t) \\ i(2b-t) & t\sqrt{1-ut} \end{bmatrix}, \tag{19}$$

and $(z)_{22} = \mu(iq)_{22}$. The determinant of z equals $(\mu|\xi|\sqrt{1-t})^{\dim V^\perp}$ times

$$\det(z)_{11} = \mu^2|\xi|^2 b^{-1}\big(4\sqrt{(1-t)(1-ut)}-(2-t)^2\big). \tag{20}$$

Given $u \in\,]0,1/2[$, the unique zero $t \in\,]0,1[$ is found as the solution of Rayleigh's cubic equation [1887, (24)], namely $0 = ((t-2)^4-16(1-t)(1-ut))/t$. Define the Rayleigh wave speed $c_r = c_s\sqrt{t} \in C^\infty(X)$. Set $p(\xi) = c_r|\xi|$. The characteristic variety Σ equals $\{p(\xi) = 1\}$. Thus (U) and (E1) hold. Obviously, $i(2b-t)\nu + t\sqrt{1-t}\,\hat{\xi} \in \ker z(\xi)$, $\xi \in \Sigma$. Observe that

$$2(2b-t) = t(2-t) \quad \text{on } \Sigma. \tag{21}$$

Thus

$$i(2-t)\nu + 2\sqrt{1-t}\,\hat{\xi} \in \ker z, \quad t = (c_r/c_s)^2, \tag{22}$$

is a nowhere vanishing section of the kernel bundle. Hence also (E2) holds. This example is of course well-known.

Remark. The identity (11) goes back to Barnett and Lothe; compare [Lothe and Barnett 1976, (3.18)]. It is key to proving, in dimension three, the uniqueness of subsonic traction-free surface waves [Barnett and Lothe 1985, Theorem 8]. The second assumption in Proposition 6 is needed to prove the existence of Rayleigh surface waves. Compare with Theorem 12 of the same reference, where existence criteria are given in terms of the so-called limiting velocity which corresponds to the boundary of the elliptic region. See [Nakamura 1991, Theorem 2.2] for the Barnett–Lothe condition in a microlocal setting, and the real principal type property of the Lopatinski matrix it entails. See [Tanuma 2007] for a recent exposition of Barnett–Lothe theory, and for a treatment of isotropic and transversely isotropic media.

3. Connections and geometric symbols

The elasticity operator is defined in terms of the Levi-Civita connection and of the elasticity tensor. We use the geometric pseudodifferential calculus of the Appendix to define and compute the leading symbol of the elasticity operator. The leading symbol includes the principal and the subprincipal level. The calculus depends on the choice of connections.

Equip M with the Levi-Civita connection of g. Let exp denote its exponential map. If $x, y \in M$, then denote by $[y \leftarrow x]$ the shortest geodesic segment from x to y, assuming its interior does not intersect the boundary, and that it is unique.

Let $E \to M$ be a (complex) vector bundle with connection ∇^E. Denote by $\tau^E_\gamma \in \mathrm{End}(E_x, E_y)$ the parallel transport map along a given curve γ in M from x to y, e.g., $\tau^E_{[y\leftarrow x]}$. The connection can be recovered from its parallel transport maps:

$$\nabla^E_v s(x) = \frac{\mathrm{d}}{\mathrm{d}t}\Big|_{t=0} \tau^E_{[x\leftarrow \exp_x tv]} s(\exp_x tv). \tag{23}$$

Denote by $\pi^* E \to T^* M$ the pullback of E to the cotangent bundle $\pi : T^* M \to M$. Let a be a smooth section of $\pi^* E \to T^* M$. Following [Sharafutdinov 2004; 2005], we introduce the vertical and the horizontal covariant derivative of a. The vertical derivative

$${}^v\nabla a(x, \xi) \in E_x \otimes T_x M,$$

at $\xi \in T^*_x M$, is the derivative of the map $T^*_x M \to E_x$, $\xi \mapsto a(x, \xi)$. The definition of the vertical derivative depends only on the linear structure of the fibers of $T^* M$. The horizontal derivative ${}^h\nabla a(x, \xi) \in E_x \otimes T^*_x M$ is the derivative at $v = 0$ of a map $T_x M \to E_x$,

$${}^h\nabla a(x, \xi) = \frac{\partial}{\partial v}\Big|_{v=0} \tau^E_{[x\leftarrow \exp_x v]} a(\exp_x v, \tau^{T^*M}_{[\exp_x v\leftarrow x]} \xi). \tag{24}$$

The horizontal derivative depends on the Riemannian structure and on the connection ∇^E. In the scalar case, $E = \mathbb{C}$, in local coordinates,

$${}^h\nabla a(x, \xi) = \big(\partial_{x_j} a(x, \xi) + \Gamma^k_{ij}(x)\xi_k \partial_{\xi_i} a(x, \xi)\big)\, \mathrm{d}x^j,$$

where Γ^k_{ij} denote the Christoffel symbols of the Levi-Civita connection. Writing a local section of $\pi^* E$ as a sum of products $a_1(x, \xi)a_2(x)$ where a_1 is scalar and a_2 a section of E one readily derives local formulas for the horizontal derivative in terms of connection coefficients. The vertical and the horizontal derivative extend to first order differential operators, ${}^v\nabla$ and ${}^h\nabla$, which map sections of $\pi^*(E \otimes T^{r,s} M)$ to sections of $\pi^*(E \otimes T^{r+1,s} M)$ and of $\pi^*(E \otimes T^{r,s+1} M)$, respectively. The operators ${}^v\nabla$ and ${}^h\nabla$ commute. It suffices to prove this when E is the trivial line bundle, $E = \mathbb{C}$. In this case the assertion is easily checked in normal coordinates.

Let $F \to M$ be another vector bundle. Let $A : C^\infty(M; E) \to C^\infty(M; F)$ be a differential operator of order m. We introduce a small parameter, $0 < h \le 1$, and we replace A by the h-differential operator $h^m A$. Then $A \in \Psi^{m,0}(M; E, F)$ as a semiclassical (pseudo-)differential operator. Refer to the Appendix for an exposition of Sharafutdinov's geometric pseudodifferential calculus in a semiclassical setting. The formula (67) for the geometric symbol, $\sigma_h(A) \in S^{m,0}$, simplifies to

$$\sigma_h(A)(x, \xi)s = A_y\big(e^{i\langle \xi, \exp_x^{-1} y\rangle/h} \tau^E_{[y\leftarrow x]} s\big)\big|_{y=x}, \tag{25}$$

where $\xi \in T^*_x M$, $s \in E_x$, and $i = \sqrt{-1}$. The geometric symbol extends by continuity to the boundary of M. In symbol computations we track the leading geometric symbol, defined before Proposition 27. In the following, the symbol of an operator is always its geometric symbol.

For the Laplace–Beltrami operator one has $\sigma_h(-h^2\Delta)(x, \xi) = |\xi|^2$. This is readily checked using normal coordinates.

From (25) and (23) deduce

$$\sigma_h(-ih\nabla^E)(\xi)e = e \otimes \xi \in E_x \otimes T^*_x M. \tag{26}$$

As before, to ease notation, we usually do not write the base point x into the arguments of tensors and symbols.

If $E \to M$ is a Hermitian vector bundle then we define, using the volume element $\mathrm{d}V_M$, the Hilbert space $L^2(E)$. Assume E and F are Hermitian vector bundles having metric connections. The leading symbol of the formal adjoint A^* of A is given by

$$\sigma_h(A^*) \equiv \sigma_h(A)^* - ih\,\mathrm{tr}\left({}^v\nabla\, {}^h\nabla\sigma_h(A)^*\right). \tag{27}$$

See Proposition 27.

Equip the bundle $E \otimes T^*M$ with the induced Hermitian structure and the induced connection. The connection is metric. Observe that the horizontal derivative of $\sigma_h(-ih\nabla^E)^*$ vanishes. Therefore, (27) and (26) imply

$$\sigma_h\big((-ih\nabla^E)^*\big)(\xi)(e \otimes \eta) = g(\xi,\eta)e, \quad \xi,\eta \in T_x^*M, e \in E_x. \tag{28}$$

By Proposition 28 the leading symbol of a composition is given as follows:

$$\sigma_h(AB) \equiv \sigma_h(A)\sigma_h(B) - ih\,\mathrm{tr}\left({}^v\nabla\sigma_h(A).\,{}^h\nabla\sigma_h(B)\right). \tag{29}$$

The trace is the contraction of the $TM \otimes T^*M$ factor which is produced by a pair of vertical and horizontal derivatives. *Note:* In (29) and below, the dot terminates a differentiated expression, serving as a closing bracket.

Let $C \in C^\infty(M; \mathrm{End}(E \otimes T^*M))$. View C as an operator acting by multiplication on sections of the bundle $E \otimes T^*M \to M$. Let ∇ denote the connection on the bundle $\mathrm{End}(E \otimes T^*M) \to M$ induced from the Levi-Civita connection and from ∇^E. Define sections $c, \mathrm{div}\, c$ of $\pi^*\,\mathrm{End}(E) \to T^*M$ as follows:

$$c(\xi)e = \langle \xi, \pi^*C(e\otimes\xi)\rangle, \quad (\mathrm{div}\, c)(\xi)e = \textstyle\sum_j \langle \eta^j, (\pi^*\nabla_{v_j}C)(e\otimes\xi)\rangle,$$

where the angular brackets denote contractions on covectors, using g. Furthermore, (v_j) and (η^j) are any dual frames of TM and T^*M.

Lemma 9. $$\sigma_h(-h^2\nabla^{E^*}\circ C\circ\nabla^E) = c - ih\,\mathrm{div}\, c + \mathcal{O}(h^2).$$

Proof. Observe that $\sigma_h(C) = \pi^*C$, and ${}^h\nabla\pi^*C = \pi^*\nabla C$. The symbol (28) is linear in ξ. Its vertical derivative is obvious. Using (29), the symbol a of $-ih\nabla^{E^*}\circ C$ is found to be

$$a(\xi)(e\otimes\eta) = \langle\xi, \pi^*C(e\otimes\eta)\rangle - ih\textstyle\sum_j\langle\eta^j, \pi^*\nabla_{v_j}C(e\otimes\eta)\rangle.$$

Here (v_j) and (η^j) are as in the definition of $\mathrm{div}\, c$. The horizontal derivative of the symbol of $-ih\nabla^E$ vanishes. Therefore,

$$\sigma_h(-h^2\nabla^{E^*}\circ C\circ\nabla^E)(\xi)e = a(\xi)\sigma_h(-ih\nabla^E)(\xi)e = a(\xi)(e\otimes\xi),$$

where we used (29). □

Now assume $E = \mathbb{C}TM$ and C the elasticity tensor. Identify

$$\mathrm{End}(\mathbb{C}T^{0,2}M) = \mathrm{End}(\mathbb{C}TM \otimes \mathbb{C}T^*M).$$

Let L the elasticity operator defined in (1). Recall from Riemannian geometry the following relation between the Levi-Civita connection and the Lie derivative:

$$(\mathcal{L}_u g)(v,w) = g(\nabla_v u, w) + g(v, \nabla_w u), \tag{30}$$

for (real) vector fields u, v, w. Using the symmetries of the elasticity tensor we get

$$L = \mathrm{Def}^* \circ C \circ \mathrm{Def} = (-i\nabla)^* \circ C \circ (-i\nabla).$$

We obtain the following corollary to Lemma 9:

$$\sigma_h(h^2 L - \rho) = c - \rho \,\mathrm{Id} - ih \operatorname{div} c + \mathcal{O}(h^2). \tag{31}$$

If the $C^{ijk\ell}$ represent C with respect to some given local coordinates, then (31) reads

$$\sigma_h(h^2 L - \rho)(\xi)^{ik} = C^{ijk\ell}\xi_j\xi_\ell - \rho\delta^{ik} - \sqrt{-1}hC^{ijk\ell}{}_{|j}\xi_\ell + \mathcal{O}(h^2).$$

The vertical bar followed by j means covariant differentiation with respect to the j-th coordinate. If the elastic medium is isotropic, the leading symbol becomes

$$\begin{aligned}&\sigma_h(h^2 L - \rho)(\xi)\\ &\quad \equiv \rho(c_p^2|\xi|^2 - 1)P(\xi) + \rho(c_s^2|\xi|^2 - 1)(\mathrm{Id} - P(\xi)) - ih\big(\nabla\lambda \otimes \xi + (\nabla\mu \otimes \xi)^* + \langle \xi, \nabla\mu\rangle \,\mathrm{Id}\big),\end{aligned} \tag{32}$$

where $P(\xi) = \hat{\xi} \otimes \hat{\xi}$ denotes the orthogonal projection to the propagation direction $\hat{\xi} = \xi/|\xi|$.

4. The elasticity operator in a boundary collar

In a boundary collar, $]-\varepsilon, 0] \times X \subset M$, we write the elasticity operator L in terms differential operators on X having coefficients which depend on $r \in I$, the negative distance to X.

Let $N(x) \in T_x M$ denote the unit exterior normal at $x \in X$. There exists $\varepsilon > 0$ such that, if we set $I =]-\varepsilon, 0]$, the exponential map of the Levi-Civita connection defines a diffeomorphism onto a neighborhood of X in M:

$$I \times X \to M, \quad (r, x) \mapsto y = \exp(rN(x)).$$

Essentially without losing generality, we assume that this map is onto M. The inverse map is $y \mapsto (r, x)$, where $-r = d(y, X)$ is the distance from y to X, and $x = p(y)$ is the unique point in X closest to y. The distance function r satisfies the (eikonal) equation $|\nabla r| = 1$ in M. Extend N to M by $N = \nabla r$. Also introduce the unit conormal field $\nu = \mathrm{d}r$. The level hypersurfaces

$$M_r = \{y \in M \,;\, r + d(y, X) = 0\}$$

are diffeomorphic to $X = M_0$. The shape operator $S = \nabla N$ is a field of symmetric endomorphisms of TM, $g(Su, v) = g(u, Sv)$. The second fundamental forms of the level hypersurfaces M_r assign $(u, v) \mapsto -g(Su, v)$ (Weingarten equation). The dependence of the metric tensor on r is given by the formula $(\mathcal{L}_N g)(v, w) = 2g(Sv, w)$. This formula follows from (30). Introduce $J \in C^\infty(I_r \times X)$, the solution of $\partial_r \log J = \operatorname{tr} S$, $J|_{r=0} = 1$. Then we have the following formula for the volume form of M:

$$\int_M f(y)\,\mathrm{d}V_M(y) = \int_I \int_X f(\exp(rN(x)))J(r, x)\,\mathrm{d}V_X(x)\,\mathrm{d}r, \tag{33}$$

$f \in C_c^\infty(M)$. See [Petersen 1998, Chapter 2] for the geometry of hypersurfaces using distance functions.

Let $E \to M$ be a vector bundle with connection ∇^E. Denote by $E_r \to M_r$ the bundles induced by the inclusions $M_r \subset M$, $r \in I$. Set $E_X = E_0$. Let $u \in C^\infty(M; E)$ be a section of E. Using parallel transport in E along the geodesics which intersect the boundary orthogonally, define $\widetilde{u} : I \to C^\infty(X; E_X)$ by

$$\widetilde{u}(r)(x) = \widetilde{u}(r, x) = \tau^E_{[x \leftarrow y]} u(y) \quad \text{if } y = \exp(rN(x)).$$

The map

$$C^\infty(M; E) \to C^\infty(I, C^\infty(X; E_X)), \quad u \mapsto \widetilde{u}, \tag{34}$$

is an isomorphism of Fréchet spaces. The isomorphism commutes with bundle operations such as tensor products and contractions.

The covariant derivative in normal direction is transformed into ∂_r under the above isomorphism:

$$\widetilde{\nabla^E_N u}(r) = \partial_r \widetilde{u}(r), \quad r \in I. \tag{35}$$

To see this, consider the geodesic $I \to M$, $r \mapsto y(r) = \exp(rN(x))$. The tangent vectors are $\dot{y}(r) = N(y(r))$. Using (23), it follows that

$$(\nabla^E_{N(y(r))} u)(y(r)) = \frac{d}{ds}\Big|_{s=r} \tau^E_{[y(r) \leftarrow y(s)]} u(y(s)) = \tau^E_{[y(r) \leftarrow x]} \frac{d}{ds}\Big|_{s=r} \widetilde{u}(s, x).$$

This implies (35). We have $\nabla_N N = SN = 0$. It follows that $\partial_r \widetilde{N} = 0$, and $\partial_r \widetilde{\nu} = 0$. Abusing notation, we write ∂_r to denote ∇^E_N.

Define $\epsilon_\nu e = e \otimes \nu$ and $\iota_\nu(e \otimes \eta) = \langle \eta, \nu \rangle e$. Notice that ϵ_ν and ι_ν commute with ∂_r.

Let $F \to M$ be a another vector bundle with a connection. Let $B : C^\infty(M; E) \to C^\infty(M; F)$ be a differential operator. Assume that B is tangential. This means, by definition, that B commutes with the distance function r, $[B, r] = 0$. Then, for every $r \in I$, B restricts to an operator $B_r : C^\infty(M_r; E_r) \to C^\infty(M_r; F_r)$, $B_r U = (Bu)|_{M_r}$, where u is a section of $E \to M$ which extends a given section U of $E_r \to M_r$. The assumption $[B, r] = 0$ implies that B_r is well-defined. Parallel transport along the geodesics orthogonal to X defines bundle isomorphisms $E_r \cong E_X$ and $F_r \cong F_X$. Via these isomorphisms the B_r's induce differential operators $B(r) : C^\infty(X; E_X) \to C^\infty(X; F_X)$, called associated with B, such that $\widetilde{Bu}(r) = B(r)\widetilde{u}(r)$, $r \in I$. Each $B(r)$ is a differential operator having coefficients which are C^∞ with respect to r. Conversely, an operator B is tangential if it is given in this way by a family of differential operators $\{B(r)\,;\, r \in I\}$ with coefficients depending smoothly on r.

Lemma 10. *Let $E \to M$ be a real vector bundle with connection ∇^E. Then*

$$\nabla^E = \epsilon_\nu \partial_r + B, \tag{36}$$

where B is tangential. Moreover, $B(0) = \nabla^{E_X}$.

Here $E \otimes T^*M$ carries the induced connection. The lemma extends, by decomposition into real and imaginary parts, to complexifications of real bundles with connections. In particular, it holds for complexified tensor bundles with the Levi-Civita connection.

Proof. Let $P^\perp, P^\parallel \in C^\infty(M; \mathrm{End}(TM))$ denote the orthogonal projectors onto the span of N and onto its orthogonal complement, $N^\perp$, respectively. Identify $E \otimes T^*M$ with $\mathrm{Hom}(TM, E)$. Let $u \in C^\infty(M; E)$. We have the following decomposition in $C^\infty(M; \mathrm{Hom}(TM, E))$:

$$\nabla^E u = (\nabla^E u) P^\perp + (\nabla^E u) P^\parallel = (\nabla^E_N u) \otimes \nu + Bu.$$

This defines B, and implies (36). Note that B is tangential. We have

$$B(0)\widetilde{u}(0) = Bu|_X = \big((\nabla^E u)P^{\|}\big)|_X = \big(\nabla^{E_X}(u|_X)\big)\big(P^{\|}|_X\big).$$

This proves the asserted formula for $B(0)$. □

Assume $E \to M$ a Hermitian bundle with a metric connection. Using (33), and the fact that parallel transport preserves inner products, we have

$$\int_M (u \mid v)_E \,\mathrm{d}V_M = \int_I \int_X (\widetilde{u} \mid \widetilde{v})_{E_X} J \,\mathrm{d}V_X \,\mathrm{d}r, \tag{37}$$

if $u, v \in C_c^\infty(M; E)$. Formal adjoints of differential operators on M are taken with respect to these inner products. The inner product of sections u and v of $E_X \to X$ is $\int_X (u \mid v)_{E_X} \,\mathrm{d}V_X$. Formal adjoints of operators $A(r)$ associated with a tangential operator A are defined with respect to this inner product.

Next we prove a formula expressing the elasticity operator L as a quadratic polynomial in $D_r = -i\partial_r$ with tangential coefficients. Now assume $E = \mathbb{C}TM$, and let B as in (36). Define tangential operators

$$A_0 = \iota_\nu C \epsilon_\nu, \quad A_1 = -i\iota_\nu CB, \quad A_2 = B^* CB.$$

The order of A_j is j. Moreover, $A_1^* = iB^* C\epsilon_\nu$.

Proposition 11. *The elasticity and traction operators defined in* (1) *are as follows*:

$$L = (D_r - i \operatorname{tr} S)(A_0 D_r + A_1) + A_1^* D_r + A_2, \quad -iT = A_0(0) D_r + A_1(0).$$

Furthermore, $A_1^*(0) = A_1(0)^*$.

Proof. Let $u, v \in C_c^\infty(M; \mathbb{C}TM)$. It follows from (30) and the symmetry properties of the elasticity tensor that

$$\int_M \big(\operatorname{Def} u \mid \operatorname{Def} v\big)_C \,\mathrm{d}V_M = \int_M \big(C\nabla u \mid \nabla v\big) \,\mathrm{d}V_M.$$

Inserting (36) and using the definition of A_j, the right-hand side equals

$$\begin{aligned}\int_M (\iota_\nu C\nabla u \mid \partial_r v) \,\mathrm{d}V_M &+ \int_M (B^* C\nabla u \mid v) \,\mathrm{d}V_M \\ &= \int_M (A_0 \partial_r u + iA_1 u \mid \partial_r v) \,\mathrm{d}V_M + \int_M (-iA_1^* \partial_r u + A_2 u \mid v) \,\mathrm{d}V_M.\end{aligned}$$

We integrate by parts, using (37), and get

$$\begin{aligned}\int_M (w \mid \partial_r v) \,\mathrm{d}V_M& \\ = \int_I \int_X (\widetilde{w} \mid \partial_r \widetilde{v}) J \,\mathrm{d}V_X \mathrm{d}r &= \int_X \big(w(0) \mid v(0)\big) \,\mathrm{d}V_X - \int_I \int_X \big((\partial_r \log J)\widetilde{w} + \partial_r \widetilde{w} \mid \widetilde{v}\big) J \,\mathrm{d}V_X \,\mathrm{d}r.\end{aligned}$$

Summing up we have

$$\begin{aligned}\int_M \big(\operatorname{Def} u \mid \operatorname{Def} v\big)_C \,\mathrm{d}V_M &= \int_M \big((D_r - i \operatorname{tr} S)(A_0 D_r + A_1)u + A_1^* D_r u + A_2 u \mid v\big) \,\mathrm{d}V_M \\ &\quad + \int_X \big(A_0(0)(\partial_r u)(0) + iA_1(0)u(0) \mid v(0)\big) \,\mathrm{d}V_X.\end{aligned}$$

Comparing with (1) the formulas for L and T follow. The last assertion follows because $J = 1$ at X. □

Next we compute the leading symbols of the operators (associated with) A_j. The symbols are r-dependent sections of $\pi^* \operatorname{End}(\mathbb{C}T_X M) \to T^*X$. Dropping tildes, the symbol of A_0 equals

$$\sigma_h(A_0) = a = c(\nu) \in C^\infty(I, C^\infty(T^*X; \pi^* \operatorname{End}(\mathbb{C}T_X M)).$$

Introduce the divergence of the acoustic tensor restricted to X as follows:

$$(\operatorname{div}_X c)(\zeta)v = \sum\nolimits_\alpha \langle \eta^\alpha, (\pi^* \nabla_{v_\alpha} C)(v \otimes \zeta)\rangle,$$

if $\zeta \in T_x^* M$, $v \in T_x M$, $x \in X$. Here (v_α) and (η^α) are any dual frames of TX and T^*X. If local coordinates are chosen such that r is one coordinate and the other coordinates are constant along the geodesics orthogonal to X, then $(\operatorname{div}_X c)(\zeta)^{ik} = C^{i\alpha k\ell}{}_{|\alpha}\zeta_\ell$. Here the summation convention is used with Latin indices referring to all coordinates, and Greek referring to all coordinates except r. We also need the contraction $\langle C, S\rangle \in C^\infty(M; \operatorname{End}(TM))$ of the elasticity tensor with the shape operator, in coordinates,

$$\langle C, S\rangle^{ik} = C^{ijk\ell} S_{j\ell}, \quad S_{j\ell} = \nu_{j|\ell}.$$

(Because $\nabla_N S = 0$ one can also write Greek indices instead of j and ℓ.)

Lemma 12. *Let a_1 and a_2 denote the principal symbols of the h-differential operators hA_1 and $h^2 A_2$, respectively. At $r = 0$: $a_1(\xi) = c(\nu, \xi)$, and $a_2(\xi) = c(\xi)$. On the leading symbol level, $\sigma_h(hA_1) = a_1$, $\sigma_h(hA_1^*) = a_1^* - iha_{1-}$, and $\sigma_h(h^2 A_2) = a_2 - iha_{2-} + \mathcal{O}(h^2)$, where, at $r = 0$,*

$$a_{1-} = (\operatorname{div}_X c)(\nu) + \pi^* \langle C, S\rangle, \quad a_{2-}(\xi) = (\operatorname{div}_X c)(\xi).$$

Proof. By Lemma 10 we have

$$hA_1(0) = \iota_\nu C \circ (-ih\nabla), \quad h^2 A_2(0) = (-ih\nabla)^* \circ C \circ (-ih\nabla),$$

where $\nabla = \nabla^{TX}$ is the Levi-Civita connection of the boundary. We compute the leading symbol of $hA_1(0)$ using the composition formula (29). Recall (26). The vertical derivative of the symbol of $\iota_\nu C$ vanishes, Hence

$$\sigma_h(hA_1)(0)(\xi) = \sigma_h(hA_1(0))(\xi) = c(\nu, \xi), \quad \xi \in T_X^* M.$$

The formula for $\sigma_h(h^2 A_2(0))$ follows from Lemma 9. In view of (27), $a_{1-} = \operatorname{tr} {}^v\nabla {}^h\nabla a_1^*$. Since $a_1^*(\xi) = c(\xi, \nu) = \langle \xi, \pi^*(C\epsilon_\nu)\rangle$ is linear in ξ, its vertical derivative is immediate. Hence

$$\operatorname{tr} {}^v\nabla {}^h\nabla a_1^* = \sum\nolimits_\alpha \langle \eta^\alpha, \pi^* \nabla_{v_\alpha}(C\epsilon_\nu)\rangle.$$

Now, $\nabla_v(C\epsilon_\nu)$ equals $(\nabla_v C)\epsilon_\nu$ plus a contraction of C with $\nabla_v \nu = Sv$, proving the formula for a_{1-}. □

If the elastic medium is isotropic, (16), then a straightforward computation shows that, at $r = 0$,

$$(\operatorname{div}_X c)(\zeta) = (\nabla\lambda \otimes \zeta) + (\nabla\mu \otimes \zeta)^* + \langle \zeta, \nabla\mu\rangle \operatorname{Id},$$
$$\langle C, S\rangle = (\lambda + \mu)S + (\mu \operatorname{tr} S) \operatorname{Id}.$$

Here $\nabla\lambda, \nabla\mu \in TX \subset T_X M$ are the gradients of the Lamé parameters restricted to X.

5. Microlocal factorization

We factorize, microlocally in the elliptic region, the h-differential operator $h^2L-\rho$ into a product with right factor hD_r-Q, where Q is a tangential h-pseudodifferential operator such that the spectrum of its principal symbol is contained in the lower half-plane, $\mathbb{C}_-$.

As in the previous section we identify M with a boundary collar $I\times X$, and sections of $\mathbb{C}TM\to M$ with r-dependent sections of $\mathbb{C}T_XM\to X$. Operators are polynomials in $D_{r/h}=hD_r$ with tangential h-(pseudo-)differential operators as coefficients. The latter are quantizations (64), $B_h=\mathrm{Op}_h(b_h)\in\Psi^{m,k}_{\mathrm{tang}}$, of tangential symbols,

$$b_h\in S^{m,k}_{\mathrm{tang}}=C^\infty(I,S^{m,k}(T^*X;\pi^*\,\mathrm{End}(\mathbb{C}T_XM))).$$

By Proposition 11 the principal symbol $f(s,\xi)=c(\xi+s\nu)-\rho$ of $h^2L-\rho$ at $\xi+s\nu$ is a second order polynomial in s. View s as the symbol of $D_{r/h}$. The coefficients are h-independent tangential symbols. By (9), there exists a constant $\delta>0$ such that

$$f(s,\xi)\geq\delta(1+|s|^2+|\xi|^2)\,\mathrm{Id},\quad s\in\mathbb{R},\tag{38}$$

holds if ξ is sufficiently large. If $F\subset\mathscr{E}$ is closed and $R>0$, then $F\setminus\{|\xi|>R\}$ is compact. Hence there exist $0<\varepsilon',\delta$ such that (38) holds uniformly for $(r,\xi)\in[-\varepsilon',0]\times F$. We say that a property holds at the elliptic region $\mathscr{E}$ if it is true in every open subset of $I\times\mathscr{E}$ where (38) holds uniformly.

Recall from Section 2 that we have a unique spectral factorization (10) at $\mathscr{E}$.

Lemma 13. *Let $q=q(\xi)$, $\xi\in\mathscr{E}$, the unique solution of the spectral factorization $f(s,\xi)=(s-q(\xi)^*)a(s-q(\xi))$, $\mathrm{spec}\,q(\xi)\subset\mathbb{C}_-$. Then $q\in S^1_{\mathrm{tang}}$ at $\mathscr{E}$.*

Proof. By Lemma 3 we have $aq=-\pi i f_0^{-1}+f_1f_0^{-1}$ with integrals $f_j=f_j(\xi)$ defined there. Using (38), we can estimate $f_0(\xi)=\int f(s,\xi)^{-1}\mathrm{d}s$ as follows:

$$|f_0(\xi)|\leq\int_{-\infty}^{\infty}\delta^{-1}(1+|s|^2+|\xi|^2)^{-1}\mathrm{d}s=\pi/\delta\langle\xi\rangle,$$

$\langle\xi\rangle=(1+|\xi|^2)^{1/2}$. The integrand $f(s,\xi)^{-1}$ remains integrable after applying ∂_r, ${}^h\nabla$, and ${}^v\nabla$ finitely many times. Therefore these derivatives can be interchanged with the integral. In view of the symbol properties of f, we deduce, using estimates as above, $f_0\in S^{-1}_{\mathrm{tang}}$ at $\mathscr{E}$. Using an upper bound $f(s,\xi)\leq\delta^{-1}(|s|^2+\langle\xi\rangle^2)\,\mathrm{Id}$, we derive $f_0(\xi)\geq\delta\langle\xi\rangle^{-1}\,\mathrm{Id}$, again in the sense of selfadjoint maps. Therefore f_0 is an elliptic symbol, and $f_0^{-1}\in S^1_{\mathrm{tang}}$ at $\mathscr{E}$.

Write $f_1=f_{10}+f_{11}$, where $f_{10}(\xi)=\int_{|s|\leq1}saf(s,\xi)^{-1}\mathrm{d}s$,

$$f_{11}(\xi)=\int_{|s|>1}s^{-1}\big(s^2a-f(s,\xi)\big)f(s,\xi)^{-1}\mathrm{d}s.$$

Recall that $s^2a-f(s)=-s(a_1+a_1^*)-(a_2-\rho)$. Reasoning as in the proof of $f_0\in S^{-1}_{\mathrm{tang}}$, we see that the integrand of f_{11} and its derivatives are integrable. Moreover, we deduce $f_{11}\in S^0_{\mathrm{tang}}$. It is easy to see that $f_{10}\in S^{-2}_{\mathrm{tang}}$. Therefore, at $\mathscr{E}$, $f_1\in S^0_{\mathrm{tang}}$. The lemma follows. ☐

For an h-tempered family $(u_h)\in h^{-\infty}C^{-\infty}(X)$ one defines the semiclassical wavefront set $\mathrm{WF}_h(u_h)\subset T^*X\sqcup S^*X$ [Gérard 1988; Sjöstrand and Zworski 2002]. Below we deal with operators associated to symbols which are not defined on all of T^*X but only at $\mathscr{E}$. These operators are defined microlocally in $\mathscr{E}$ by letting them operate on the subspace of distributions (u_h) which satisfy $\mathrm{WF}_h(u_h) \subset \mathscr{E}$, modulo the space $h^\infty C^\infty$.

Lemma 14. *Let q be as in Lemma 13. Microlocally at $\mathscr{E}$,*

$$h^2 L - \rho = (D_{r/h} - Q^\sharp) A_0 (D_{r/h} - Q), \tag{39}$$

where $Q, Q^\sharp \in \Psi^{1,0}_{\mathrm{tang}}$, such that $Q - \mathrm{Op}_h(q), Q^\sharp - \mathrm{Op}_h(q^*) \in \Psi^{0,-1}_{\mathrm{tang}}$. Here A_0 is as in Proposition 11.

Proof. Initially we set $Q = \mathrm{Op}_h(q)$ and $Q^\sharp = \mathrm{Op}_h(q^*)$. At $\mathscr{E}$,

$$h^2 L - \rho = (D_{r/h} - Q^\sharp) A_0 (D_{r/h} - Q) + R_1 + R_0\, D_{r/h}, \tag{40}$$

where $R_j \in \Psi^{j,-1}_{\mathrm{tang}}$. Here we used the formula for L given in Proposition 11. Observe that, if $A \in \Psi^{m,k}_{\mathrm{tang}}$, then the commutator $[D_{r/h}, A]$ belongs to $\Psi^{m,k-1}_{\mathrm{tang}}$. Aiming at an inductive construction, we assume that (40) holds for some positive integer k such that $R_j \in \Psi^{j+1-k,-k}_{\mathrm{tang}}$. The spectra of q and q^* are disjoint. It follows that the equation $sq - q^* s = r$ has, at $\mathscr{E}$, for every symbol $r \in S^m$ a unique solution $s \in S^{m-1}$. Applying this construction to the principal symbols of the R_j's, we find operators $S_j \in \Psi^{j-k,-k}_{\mathrm{tang}}$ such that $S_j Q - Q^\sharp S_j - R_j$ lies in $\Psi^{j-k,-k-1}_{\mathrm{tang}}$. Set

$$Q_1 = Q - A_0^{-1}(S_0 Q + S_1), \quad Q_1^\sharp = Q^\sharp + (Q^\sharp S_0 + S_1) A_0^{-1}.$$

Then

$$\begin{aligned}(D_{r/h} - Q_1^\sharp) A_0 (D_{r/h} - Q_1) = (D_{r/h} - Q^\sharp) A_0 (D_{r/h} - Q) + \big(S_0 Q - Q^\sharp S_0\big) D_{r/h} + \big(S_1 Q - Q^\sharp S_1\big)\\ + [D_{r/h}, S_0 Q + S_1] - (Q^\sharp S_0 + S_1) A_0^{-1} (S_0 Q + S_1).\end{aligned}$$

Replace Q and $Q^\sharp$ by Q_1 and $Q_1^\sharp$, respectively. By the symbol calculus, (40) holds with smaller errors, $R_j \in \Psi^{j-k,-k-1}_{\mathrm{tang}}$. The proof is completed using asymptotic summation. □

It follows from the foregoing construction that the symbol of Q is classical.

6. A Dirichlet parametrix

Microlocally at $\mathscr{E}$, we solve, constructing a parametrix, $Bf = u$, the Dirichlet problem $h^2 Lu - \rho u = 0$, $u|_X = f$. We adapt the method of [Taylor 1996, 7.12] to our setting.

Denote by

$$S^m_{\mathrm{pois}} \subset C^\infty([-1, 0], C^\infty(T^*X; \pi^* \operatorname{End}(\mathbb{C}T_X M)))$$

the space of symbols $b(s, \eta)$, $-1 \le s \le 0$, $\eta \in T^*X$, that satisfy the estimates

$$\big|\partial_s^\tau ({}^v\nabla)^j ({}^h\nabla)^\ell b(s, \eta)\big| \le C_{\tau j \ell} \langle \eta \rangle^{m+\tau-j},$$

for all nonnegative integers τ, j, and ℓ. Let $S^{m,k}_{\mathrm{pois}}$ denote the corresponding space of h-dependent symbols b_h. Observe that $g(s\langle\eta\rangle) \in S^0_{\mathrm{pois}}$ if $g(t) = |t|^j e^{\varepsilon t}$, $\varepsilon > 0$, j a nonnegative integer.

We continue to work in a collar $I \times X \subset M$. Choose a cutoff χ_0 as in (64). Let $\delta > 0$. Given $b_h \in S^{m,k}_{\mathrm{pois}}$, introduce the operator $B_h = \mathrm{Op}_{\delta,h}(b_h(r/h))$ by setting

$$B_h f(r, y) = (2\pi h)^{-n} \int\limits_{T_y^*} \int\limits_{T_y} e^{-i\langle \eta, v\rangle/h + \delta r\langle\eta\rangle/h} \chi_0(y, v) b_h(r/h, y, \eta) \tau^{\mathbb{C}T_X M}_{[y\leftarrow \exp_y v]} f(\exp_y v)\,\mathrm{d}v\,\mathrm{d}\eta, \quad (41)$$

for $r \in I$, $n = \dim X$. We call B_h a Poisson operator with symbol b_h and (exponential) decay δ. The arguments in [Taylor 1996, Chapter 7, Proposition 12.4] apply to give $B_h : L^2(X) \to H_h^{-m+1/2}(I \times X)$ with norm $\mathbb{O}(h^{-k+1/2})$. (The Sobolev spaces H^s_h are defined using hD instead of D.) If $0 < \delta' < \delta$ and $j \in \mathbb{N}$, then

$$r^j B_h \in \mathrm{Op}_{\delta',h} S^{m-j,k-j}_{\mathrm{pois}}.$$

Moreover, $B_h f \in C^\infty$ in $r < 0$, and $B_h f(r)$ decays together with its derivatives as $e^{\delta' r/h}$, uniformly if f ranges in a bounded subset of $L^2(X)$. We call h-dependent operators negligible if they have Schwartz kernels which are smooth and $\mathbb{O}_{C^\infty(M\times X)}(h^\infty)$. We write $A \equiv B$ if and only if $A - B$ is negligible. Note that B_h in (41) is negligible if there exists $\epsilon > 0$ such that $b_h(s, \eta) = 0$ if $-\epsilon < s \le 0$.

We need to handle the composition of a Poisson operator with a tangential operator. The following lemma deals with this when the symbols are classical, i.e., possess asymptotic expansions in powers of h.

Lemma 15. *Let $0 < \delta' < \delta$. Let $A = \mathrm{Op}_h a(r)$ and $B = \mathrm{Op}_{\delta,h} b(r/h)$, where $a = a(r, \eta) \in S^1_{\mathrm{tang}}$ and $b(s, \eta) \in S^m_{\mathrm{pois}}$ are h-independent symbols. Then*

$$AB \equiv \mathrm{Op}_{\delta',h} c(r/h),$$

where $c = c_h \in S^{m+1,0}_{\mathrm{pois}}$ has an asymptotic expansion $c \sim \sum_{j\ge0} h^j c_j$, $c_j \in S^{m+1-j}_{\mathrm{pois}}$. The principal term equals

$$c_0(s, \eta) = a(0, \eta) b(s, \eta) e^{(\delta-\delta')s\langle\eta\rangle}.$$

Proof. Using Taylor expansions, $a(r, \eta) = \sum_{j<N} r^j a_j(\eta) + r^N a'_N(r, \eta)$, and the properties of $r^j B$ noted above, we may assume without loss of generality that a does not depend on r. Arguing as in the proof of Proposition 28 we can write, at least formally, $AB = \mathrm{Op}_{0,h} \tilde{c}(r/h)$, where

$$\tilde{c}(s,x,\xi) = (2\pi h)^{-2n} \int\limits_{T_x\times T_x^*\times T_x\times T_x^*} e^{i\varphi/h} a(x,\eta) \tau^{\pi^*\mathrm{End}(\mathbb{C}T_X M)}_{[x\leftarrow y]} b(s,y,\zeta) e^{\delta s\langle\zeta\rangle} M(x,w+v,v)\,\mathrm{d}(v,\eta,w,\vartheta),$$

φ as in (72). We use the standard arguments in handling compositions of symbols: dyadic decompositions and the method of (non-)stationary phase. We infer that there exist $\epsilon > 0$ and $d_j \in S^{m+1-j}_{\mathrm{pois}}$, $d_0(s, \eta) = a(\eta) b(s, \eta)$, such that for every N,

$$\tilde{c}(s, \eta) = \Bigl(\sum_{j<3N} h^j d_j(s, \eta)\Bigr) e^{\delta s\langle\eta\rangle} + \tilde{d}_{Nh}(s, \eta) e^{\epsilon s\langle\eta\rangle},$$

where $\tilde{d}_{Nh} \in S^{m+1-N,-N}_{\mathrm{pois}}$. Observe that $\langle\xi\rangle/\langle\eta\rangle$ is uniformly bounded from below if ξ and η range in the same dyadic shell. Above we have chosen ϵ less than δ times this bound. Define $c_h(s, \eta)$ as the product of an asymptotic sum $\sum_{j\ge0} h^j d_j(s, \eta)$ with the symbol $e^{(\delta-\delta')s\langle\eta\rangle} \in S^0_{\mathrm{pois}}$. It follows that $AB - \mathrm{Op}_{\delta',h} c(r/h)$ belongs to $\mathrm{Op}_{\epsilon,h} S^{m+1-N,-N}_{\mathrm{pois}}$ for every N. Thus $AB \equiv \mathrm{Op}_{\delta',h} c(r/h)$. ☐

Let q and Q be as in Lemma 14. If $\eta \in \mathscr{E}$ ranges in a set having a positive distance to the complement of the elliptic region, then there exist positive constants δ_0 and M such that

$$|e^{siq(0,\eta)}| \le M e^{s\delta_0\langle\eta\rangle}, \quad s \le 0. \tag{42}$$

This follows from the fact that the spectrum of $q(0,\eta)/\langle\eta\rangle$ is contained in a compact subset of the lower half-plane then. We shall solve $(D_{r/h} - Q)B \equiv 0$, $B|_{r=0} = \mathrm{Id}$, microlocally at $\mathscr{E}$. On the symbol level we have to solve linear ordinary differential equations with constant coefficient matrices. The following assertions are true microlocally in $\mathscr{E}$ where (42) holds.

Lemma 16. *Let $0 < \delta < \delta_0$. Let $r \in S^{1+m}_{\mathrm{pois}}$ and $v \in S^m$. Let $b(s,\eta)$ be the solution of the initial value problem*

$$\partial_s b(s,\eta) = \big(iq(0,\eta) - \delta\langle\eta\rangle\big)b(s,\eta) + r(s,\eta), \quad -1 < s \le 0, \tag{43}$$

and $b(0,\eta) = v(\eta)$. Then $b(s,\eta) \in S^m_{\mathrm{pois}}$.

Proof. Note that the coefficient matrix of (43) does not depend on s. Representing b by Duhamel's formula and using (42) we derive the estimate

$$|b(s,\eta)| \le M|v(\eta)| + M\int_s^0 e^{(\delta_0-\delta)s\langle\eta\rangle}|r(s,\eta)|\,\mathrm{d}s \le M|v(\eta)| + \frac{M}{\delta_0-\delta}\sup_{s\le 0}|r(s,\eta)|/\langle\eta\rangle.$$

Moreover, we can estimate $\partial_s b(s,\eta)$ by estimating the right-hand side of (43). Differentiating (43) we derive linear ordinary differential equations for $\partial_s^\tau({}^v\nabla)^j({}^h\nabla)^\ell b(s,\eta)$. These equations are of the same structure as (43) with the same coefficient matrix. The asserted symbol estimates are obtained recursively. □

Proposition 17. *Let $0 < \delta < \delta_0$, and $\epsilon > 0$. There exists $B \in \mathrm{Op}_{\delta,h} S^{0,0}_{\mathrm{pois}}$ with Schwartz kernel supported in $-\epsilon < s \le 0$, such that, microlocally at $\mathscr{E}$, $(D_{r/h} - Q)B \equiv 0$ and $B|_{r=0} = \mathrm{Id}$. Moreover, $(h^2L - \rho)B \equiv 0$.*

Proof. It follows from Lemma 15 that, for a classical symbol $b \in S^{m,k}_{\mathrm{pois}}$, $0 < \delta' < \delta$, modulo negligible operators, the composition

$$(D_{r/h} - Q)\,\mathrm{Op}_{\delta,h}\, b(r/h)$$

equals $\mathrm{Op}_{\delta',h}\, c(r/h)$, $c \in S^{m+1,k}_{\mathrm{pois}}$. Moreover, c is classical, and, modulo $S^{m,k-1}_{\mathrm{pois}}$,

$$c(s,\eta) \equiv \big(-i\partial_s b(s,\eta) - i\delta\langle\eta\rangle b(s,\eta) - q(0,\eta)b(s,\eta)\big)e^{(\delta-\delta')s\langle\eta\rangle}.$$

Fix a sequence (δ_j), $\delta < \delta_{j+1} < \delta_j$. Using Lemmas 15 and 16 we recursively find h-independent symbols $b_j \in S^{1-j}_{\mathrm{pois}}$, $b_1|_{r=0} = \mathrm{Id}$, $b_j|_{r=0} = 0$ if $j > 1$, such that $B_j = h^{j-1}\,\mathrm{Op}_{\delta_j,h}\, b_j(r/h)$ satisfy

$$(D_{r/h} - Q)(B_1 + \cdots + B_j) \in \mathrm{Op}_{\delta',h} S^{1-j,-j}_{\mathrm{pois}}, \quad \delta_{j+1} < \delta' < \delta_j.$$

Now B is constructed using asymptotic summation. The last assertion follows from the factorization (39). □

7. The displacement-to-traction operator

In this section we deal with operators on the boundary X. Therefore, in the following, operators and symbols are, as a rule, evaluated at $r=0$.

Let B denote the Dirichlet parametrix given in Proposition 17 and T the traction defined in (1). The operator $Z=hTB$ is called the semiclassical displacement-to-traction operator, or Neumann operator, at $\mathscr{E}$. By Propositions 11 and 17 we have, if $\mathrm{WF}_h(f)\subset\mathscr{E}$,

$$Zf=(iA_0D_{r/h}Bf+ihA_1Bf)|_X=iA_0(0)Q(0)f+ihA_1(0)f.$$

Therefore, $Z=iA_0Q+ihA_1$, and Z is, microlocally in $\mathscr{E}$, a pseudodifferential operator of class $\Psi^{1,0}$. The symbol of Z is classical since the symbols of A_j and Q are.

Lemma 18. *The displacement-to-traction operator Z is, in $\mathscr{E}$, up to a negligible operator, formally selfadjoint. The principal symbol of Z equals the surface impedance tensor*

$$z=i(aq+a_1)\in S^1(\mathscr{E};\pi^*\operatorname{End}(\mathbb{C}T_XM)). \tag{44}$$

The leading symbol of Z is $z+hz_-$, where $z_-\in S^0$,

$$z_-q-q^*z_-=i\operatorname{tr}(S)z+i\partial_rz-a_{2-}-a_{1-}q+\operatorname{tr}\left({}^v\nabla q^*.a\,{}^h\nabla q\right). \tag{45}$$

Proof. Let $f_1,f_2\in L^2(X;\mathbb{C}T_XM)$, $\mathrm{WF}_h(f_j)\subset\mathscr{E}$, and set $u_j=Bf_j$. By (1),

$$\int_X(Zf_1\mid f_2)\,\mathrm{d}V_X-\int_X(f_1\mid Zf_2)\,\mathrm{d}V_X=h^{-1}\int_M(u_1\mid h^2Lu_2-\rho u_2)-(h^2Lu_1-\rho u_1\mid u_2)\,\mathrm{d}V_M.$$

It follows from Proposition 17 that the right-hand side is $\mathbb{O}(h^\infty)$, uniformly if the f_j's range in a bounded set and have h-wavefronts contained in a common closed subset of $\mathscr{E}$. Thus $Z^*=Z$ in $\mathscr{E}$. Recalling $Z=iA_0Q+ihA_1$, we infer from the symbol calculus that $z=i(aq+a_1)$ is the principal symbol.

It remains to prove the formula for z_-. Write the leading symbols of Q and $Q^\sharp$ as $q+hq_-$ and $q^*+hq^\sharp_-$, respectively. It is easy to see that $z_-=iaq_-$. Recall the formula for L in Proposition 11. The factorization (39) is equivalent to

$$(D_{r/h}-ih\operatorname{tr}(S))hA_1+(hA_1^*-ih\operatorname{tr}(S)A_0)D_{r/h}+h^2A_2-\rho=-D_{r/h}A_0Q-Q^\sharp A_0D_{r/h}+Q^\sharp A_0Q.$$

This in turn is equivalent to the following two equations of tangential operators:

$$hA_1+hA_1^*-ih\operatorname{tr}(S)A_0+A_0Q+Q^\sharp A_0=0,$$
$$[D_{r/h},A_0Q+hA_1]-ih\operatorname{tr}(S)hA_1+h^2A_2-\rho-Q^\sharp A_0Q=0.$$

On the principal symbol level these equations become $a_1+a_1^*+aq+q^*a=0$ and $a_2-\rho-q^*aq=0$. These equations agree with (10). On the leading symbol level the equations become, after division by h,

$$-ia_{1-}-i\operatorname{tr}(S)a+aq_-+q^\sharp_-a-i\operatorname{tr}\left({}^v\nabla q^*.{}^h\nabla a\right)=0,$$
$$-\partial_rz-i\operatorname{tr}(S)a_1-ia_{2-}-q^*aq_--q^\sharp_-aq+i\operatorname{tr}\left({}^v\nabla q^*.{}^h\nabla aq\right)=0.$$

Elimination of $q^\sharp_-$ from these equations gives

$$(aq_-)q-q^*(aq_-)=ia_{1-}q+\operatorname{tr}(S)z+\partial_rz+ia_{2-}-i\operatorname{tr}\left({}^v\nabla q^*.a\,{}^h\nabla q\right).$$

Formula (45) for $z_- = iaq_-$ follows. □

In principle z_- is found as the unique solution of the linear Equation (45). The right-hand side of the equation consists of known quantities and their first order derivatives. Refer to Section 10 for an algorithm computing z_- if the elastic medium is isotropic.

8. Diagonalization of Z

Assume (U) and (E1). By Proposition 6 the kernel $\ker z$ defines a line bundle over the characteristic variety $\Sigma = p^{-1}(1)$ of the surface impedance tensor z. Since zero is a simple eigenvalue of z at Σ, there exist $\epsilon > 0$ and an open neighborhood $K \subset \mathscr{E}$ of Σ such that $z(\xi)$, $\xi \in K$, has exactly one eigenvalue $\lambda_0(\xi)$ of modulus $< \epsilon$. (In the following, K is to be replaced by a smaller neighborhood when necessary.) The line bundle $E_0 = \ker(z - \lambda_0) \to K$ is a subbundle of $\pi^*\mathbb{C}T_X M = \mathrm{Hom}(\mathbb{C}, \pi^*\mathbb{C}T_X M)$. The orthoprojector onto this bundle is given by a contour integral, $u_0 = (2\pi i)^{-1} \oint_{|\lambda|=\epsilon} (\lambda - z)^{-1} \mathrm{d}\lambda$. Denote by $u_1 = \mathrm{Id} - u_0$ the orthoprojector onto the orthogonal bundle, E_1.

Assume also (E2). Choose a unit section v of $\ker z \to \Sigma$, $|v| = 1$. Using u_0, extend v to a unit section of $E_0 \to K$. Call this section also v. Clearly, $u_0 = v \otimes v^*$. If $R \in \Psi^{0,0}$ denotes the inverse of a square root of the scalar operator $\mathrm{Op}_h(v)^* \,\mathrm{Op}_h(v)$, then $V = \mathrm{Op}_h(v) R$ satisfies $V^* V = \mathrm{Id}$, i.e., V is an isometry.

Lemma 19. *Choose $V \in \Psi^{0,0}(K; \mathbb{C}, \mathbb{C}T_X M)$, with principal symbol v, such that $V^*V = \mathrm{Id}$. Set $U_0 = VV^*$, $U_1 = \mathrm{Id} - U_0$. There exist $B \in \Psi^{-1,-2}(X; \mathbb{C}T_X M)$, $B^* = B$, and $R \in \Psi^{-1,-1}(X; \mathbb{C}T_X M)$, $R^* + R = 0$, such that, microlocally in K,*

$$(\mathrm{Id} - R^*) Z (\mathrm{Id} - R) = U_0 (Z + B) U_0 + U_1 (Z + B) U_1. \tag{46}$$

In particular,

$$(\mathrm{Id} - R^*) Z (\mathrm{Id} - R) V = V V^* (Z + B) V. \tag{47}$$

The leading symbol of the scalar operator $V^*(Z + B)V \in \Psi^{1,0}$ equals

$$\lambda_0 + h(z_- v \mid v) - ih \,\mathrm{tr}\big(v^* \, {}^v\nabla z . {}^h\nabla v + {}^v\nabla v^* . {}^h\nabla \lambda_0 . v\big). \tag{48}$$

Here, as in Lemma 18, $z + hz_-$ denotes the leading symbol of Z.

Proof. To prove (46) we adopt ideas from [Stefanov 2000]. The operators U_0 and U_1 are orthogonal projectors, $U_j^* = U_j = U_j^2$, and $U_1 U_0 = 0$. Write

$$Z = U_0 Z U_0 + U_1 Z U_1 + B,$$

where $B = U_0 Z U_1 + U_1 Z U_0$. Since $u_j z = z u_j$ and $u_1 u_0 = 0$ we have $B \in \Psi^{0,-1}$. Let hb, with $b = b^* \in S^0$, denote the principal symbol of B. Define the section $z_j = z|_{E_j}$ of $\mathrm{End}(E_j)$. The spectra of z_0 and z_1 are disjoint. Therefore the Sylvester equation $s z_0 - z_1 s = u_1 b u_0$ has a unique solution s which is a section of $\mathrm{Hom}(E_0, E_1)$. We extend s to a section of $\mathrm{End}(\pi^*\mathbb{C}T_X M)$ by $s = u_1 s u_0$. Then $sz - zs = u_1 b u_0$, and $s \in S^{-1}$. Define $S = \mathrm{Op}_h(hs)$ and $R = U_0 S^* U_1 - U_1 S U_0$. Then, $R^* = -R$ and $B = U_0 B U_1 + U_1 B U_0 \equiv R^* Z + Z R$ modulo $\Psi^{-1,-2}$. Therefore, with a different $B \in \Psi^{-N+1,-N}$, $N = 2$, and $Z_0 = Z_1 = Z$, we have

$$(\mathrm{Id} - R^*) Z (\mathrm{Id} - R) = U_0 Z_0 U_0 + U_1 Z_1 U_1 + B. \tag{49}$$

If $N \geq 2$ then, using the same construction as before, we find $R_1 \in \Psi^{-N,-N}$, $R_1^* = -R_1$ such that $U_0 B U_1 + U_1 B U_0 \equiv R_1^* Z + Z R_1$ modulo $\Psi^{-N,-N-1}$. Hence we get (49) with R and Z_j replaced by $R + R_1$ and $Z_j + B$, respectively. The new error B belongs to $\Psi^{-N,-N-1}$. Iterating this construction and using asymptotic summation (46) follows. Since $U_0 V = V$, (46) implies (47).

Observe that the leading symbols of $V^*(Z+B)V$ and V^*ZV are equal. The principal symbol equals $(v \mid zv) = \lambda_0$ because $|v| = 1$. We write the leading symbol of V as $(1 + h\gamma)v + hw$, where $v^* w = (w \mid v) = 0$. Note that $(v \mid zw) = 0$. A straightforward symbol computation, using (68) and (71), gives

$$\sigma_h(V^*ZV) \equiv \lambda_0 + h(z_{-}v \mid v) + h(\gamma + \overline{\gamma})\lambda_0 - ih \operatorname{tr}\bigl(v^* \, {}^v\nabla z. {}^h\nabla v + {}^v\nabla \, {}^h\nabla v^*.zv + {}^v\nabla v^*. {}^h\nabla zv\bigr)$$

modulo $\mathbb{O}(h^2)$. From $V^*V = 1$ it follows that the leading symbol of V^*V equals unity. Since $|v|^2 = 1$ is the principal symbol, this implies

$$h(\gamma + \overline{\gamma}) - ih \operatorname{tr}\bigl({}^v\nabla \, {}^h\nabla v^*.v + {}^v\nabla v^*. {}^h\nabla v\bigr) = 0.$$

Therefore the expression for the symbol of V^*ZV simplifies to

$$\sigma_h(V^*ZV) \equiv \lambda_0 + h(z_{-}v \mid v) + ih \operatorname{tr}\bigl(\lambda_0 \, {}^v\nabla v^*. {}^h\nabla v - v^* \, {}^v\nabla z. {}^h\nabla v - {}^v\nabla v^*. {}^h\nabla zv\bigr)$$

modulo $\mathbb{O}(h^2)$. Using ${}^h\nabla zv = \lambda_0 \, {}^h\nabla v + {}^h\nabla\lambda_0.v$ we deduce (48). □

Denote by Ψ^m_{phg} the class of h-independent pseudodifferential operators A with polyhomogeneous symbols, $a \sim \sum_{j \leq m} a_j$, a_j homogeneous of degree j. When regarded as an h-dependent operator, $A \in \Psi^{m,m}$ has the classical symbol $\sum_{j \leq m} h^{-j} a_j$. In the next lemma, following [Popov and Vodev 1999] and [Stefanov 2000], we use this relation to conjugate the scalar operator constructed in Lemma 19 into $hP - 1$, where P is h-independent.

Recall that $\Omega^{1/2} \to X$ denotes the bundle of half-densities.

Lemma 20. *There is a selfadjoint operator $P \in \Psi^1_{\text{phg}}(X; \Omega^{1/2})$ with principal symbol p, and an operator $A \in \Psi^{0,0}$ from half-density sections to scalar functions, elliptic near Σ, such that $A^*V^*(Z+B)VA = hP - 1$ in a neighborhood of Σ. The subprincipal symbol of P equals, on Σ,*

$$p_{\text{sub}} = (\dot{z}v \mid v)^{-1}\bigl(\operatorname{Re}(z_{-}v \mid v) + \operatorname{Im}\operatorname{tr}(v^* \, {}^v\nabla z. {}^h\nabla v)\bigr) + \operatorname{Im}\operatorname{tr}({}^h\nabla p. {}^v\nabla v^*.v). \tag{50}$$

Here $\dot{z}$ denotes the radial derivative of z. If instead of v another unit section $\tilde{v} = e^{i\varphi}v$ of $\ker z \to \Sigma$ *is used to define V, and thus P, then the principal symbol of P remains unchanged, whereas the subprincipal changes to $\tilde{p}_{\text{sub}} = p_{\text{sub}} + \{p, \varphi\}$ on Σ. Here $\{p, \varphi\}$ denotes the Poisson bracket.*

Obviously, P is elliptic and bounded from below.

Proof. The radial derivatives of p and of $\lambda_0 = (zv \mid v)$ are, at Σ, equal to 1 and $(\dot{z}v \mid v) > 0$, respectively. Therefore, near Σ, $a_0^2\lambda_0 = p - 1$ for some $a_0 \in C^\infty$, $a_0 > 0$. Set $\tilde{Z} = A_0^*V^*(Z+B)VA_0$, $A_0 = \operatorname{Op}_h(a_0)$. Choose $\tilde{P}_1 \in \Psi^{1,0}$ (formally) selfadjoint with leading symbol $p - ih\operatorname{tr}({}^v\nabla \, {}^h\nabla p)/2$. The selfadjoint operators $\tilde{Z}$ and $\tilde{P}_1 - 1$ have the same principal symbol, $p - 1$. Therefore, the imaginary parts of their leading symbols are equal. It follows that the principal symbol q_0 of $\tilde{Q}_0 = \tilde{Z} - (\tilde{P}_1 - 1) \in \Psi^{0,0}$ equals, on Σ, $a_0^2 = (\dot{z}v \mid v)^{-1}$ times the real part of the coefficient of h in (48).

Define $p_0 \in C^\infty(T^*X\setminus 0)$, homogeneous of degree 0, and $r_{-1} \in S^{-1}$ such that $q_0 = p_0 + 2(p-1)r_{-1}$ holds in a neighborhood of Σ. Then

$$(1 - h\,\mathrm{Op}_h(r_{-1})^*)\tilde{Z}(1 - h\,\mathrm{Op}_h(r_{-1})) = \tilde{P}_1 + h\tilde{P}_0 - 1 + h\tilde{Q}_{-1},$$

where $\tilde{P}_0$ is selfadjoint with principal symbol p_0. Proceeding inductively, we obtain selfadjoint operators $\tilde{P}_j \in \Psi^{j,0}$ with classical symbols such that, for $N < 1$,

$$(1 - hR_N^*)\tilde{Z}(1 - hR_N) = h \sum_{N<j\le 1} h^{-j}\tilde{P}_j - 1 + h^{-N}\tilde{Q}_N,$$

where $\tilde{Q}_N \in \Psi^{N,0}$, $R_N \in \Psi^{-1,0}$. Therefore, there is an h-independent operator $P \in \Psi^1_{\mathrm{phg}}$ such that $(1 - hR^*)\tilde{Z}(1 - hR) = hP - 1$ near Σ. Moreover, $P \equiv \tilde{P}_1 + h\tilde{P}_0$ modulo $\Psi^{-1,-2}$. The symbol of P equals $p - i\,\mathrm{tr}({}^v\nabla\, {}^h\nabla p)/2 + p_0$ modulo S^{-1}. It follows from Corollary 29, or rather its analogue for h-independent operators, that p is the principal symbol of P and $p_{\mathrm{sub}} = p_0$ its subprincipal symbol. By construction $p_0 = q_0$ on Σ. Formula (50) follows from the formula for q_0 mentioned earlier.

Note that $\{p, \varphi\} = \mathrm{tr}\big({}^v\nabla p.{}^h\nabla\varphi - {}^h\nabla p.{}^v\nabla\varphi\big)$. The last assertion of the lemma follows from (50), using $v^*\,{}^v\nabla z.v = {}^v\nabla\lambda_0$. □

Proof of Theorem 1. The following assertions hold microlocally in a neighborhood of Σ. It follows from Lemmas 19 and 20 that

$$(\mathrm{Id} - R^*)Z(\mathrm{Id} - R)VA = VA^{-*}(hP - 1),$$

where A^{-*} denotes a parametrix of A^*. Define $J_h = (\mathrm{Id} - R)VA$ and $\tilde{J}_h = (\mathrm{Id} - R^*)^{-1}VA^{-*}$. We have $J_h, \tilde{J}_h \in \Psi^{0,0}$, $\tilde{J}_h - J_h \in \Psi^{-1,-1}$. Moreover, $J_h^* J_h$ is elliptic. By definition of Z, $TB_hJ_h = \tilde{J}_h(P - h^{-1})$, where B_h is the Dirichlet parametrix given in Proposition 17. Combining the results in Section 6 with Lemmas 19 and 20, the theorem follows. □

9. Construction of quasimodes

Given P of Theorem 1 we associate to the sequence of positive eigenvalues of P a sequence of quasimodes of L_T. We follow [Stefanov 2000, Section 4], differing in some details, however.

Let P, B_h, and J_h as in Theorem 1. Assume given a sequence of quasimodes, (μ_j), with almost orthogonal quasimodes states:

$$Pf_j - \mu_j f_j = \mathbb{O}_{C^\infty}(h_j^\infty), \quad (f_j \mid f_k) - \delta_{jk} = \mathbb{O}((h_j + h_k)^\infty), \tag{51}$$

$f_j \in C^\infty(X; \Omega^{1/2})$, $0 < \mu_j \le \mu_{j+1} \to \infty$, $h_j = \mu_j^{-1}$.

We define quasimode states for the traction-free boundary problem. By Theorem 1 the traction $t_j = TB_{h_j}J_{h_j}f_j = \mathbb{O}_{C^\infty}(h_j^\infty)$. Choose $u_j' = \mathbb{O}_{C^\infty}(h_j^\infty)$ satisfying $A_0(0)\partial_r u_j'|_X + t_j = 0$ and $u_j'|_X = 0$. Define $u_j \in C_c^\infty(M; \mathbb{C}TM)$,

$$u_j = h_j^{-1/2}\big(B_{h_j}J_{h_j}f_j + u_j'\big). \tag{52}$$

By Theorem 1,

$$Lu_j - \mu_j^2\rho u_j = \mathbb{O}_{C^\infty}(h_j^\infty), \quad Tu_j = 0, \tag{53}$$

and $\|u_j\|_{L^2} = \mathbb{O}(1)$. We can assume that the u_j are supported in a given neighborhood of X. Using the ellipticity of L, we deduce $\|u_j\|_{H^2} = \mathbb{O}(h_j^{-2})$.

To go from quasimodes to eigenvalues or, in scattering theory, to resonances, it is desirable to be able to decompose the quasimodes into well-separated clusters. In addition, the quasimode states of each cluster should be linearly independent, and remain so after applying small perturbations.

Proposition 21. *Let the assumptions of Theorem 1 hold. Assume given quasimodes $\mu_j = h_j^{-1} > 0$ of P as in* (51), *and define u_j as in* (52). *Then* (53) *holds. Let $m > \dim X$. There exist $\delta > 0$ and a covering of $\{\mu_j\}$ by a sequence of intervals $[a_k, b_k] \subset \mathbb{R}_+$, such that*

$$b_k + 2\delta b_k^{-m-\dim X} < a_{k+1}, \quad b_k - a_k < b_k^{-m}.$$

Let $w_j \in H^2(M; \mathbb{C}TM)$ be such that, for some $N \geq 0$,

$$\|w_j\|_{H^2} = \mathbb{O}(h_j^{-2-N}), \quad w_j - u_j = \mathbb{O}_{L^2}(h_j^{2\dim X+N}).$$

Then, for large k, $\{w_j\}_{a_k \leq \mu_j \leq b_k}$ is linearly independent.

Proof. Property (53) is clear by the arguments already given.

It is well-known that a quasimode sequence (51) is asymptotic to a subsequence of the sequence of eigenvalues of P. The latter satisfies the Weyl asymptotics. Hence we have a Weyl estimate $j \leq C\mu_j^{\dim X}$. It follows that every interval $[a, b]$, $1 \leq b$, of length $> L$ has a subinterval of length $\geq Lb^{-\dim X}/C$ containing no quasimode μ_j. The existence of intervals $[a_k, b_k]$ having the stated properties follows from this observation. Compare [Stefanov 1999, Proof of Theorem 2]. Define the set of indices of the k-th cluster: $I_k = \{j\ ;\ \mu_j \in [a_k, b_k]\}$.

Choose a left inverse $K_h \in \Psi^{0,0}(X; \mathbb{C}T_X M, \Omega^{1/2})$ of J_h, $K_h J_h = \mathrm{Id}$ at Σ. Since $J_h^* J_h$ is elliptic at Σ, K_h is readily found.

Denote by $\gamma : v \mapsto v|_X$ the trace map. By (52), $h_j^{1/2}\gamma u_j = J_{h_j} f_j + \gamma u_j'$. From (51) it follows that $\mathrm{WF}_{h_j} f_j \subset \Sigma$. Therefore,

$$h_j^{1/2} K_{h_j}\gamma u_j = f_j + \mathbb{O}_{C^\infty}(h_j^\infty).$$

By the remark after Lemma 26 we can assume that there exists a constant C such that for all $j, \ell \in I_k$, $k \in \mathbb{N}$,

$$\|K_{h_\ell} - K_{h_j}\|_{L^2 \to L^2} \leq Cb_k |h_\ell - h_j|.$$

Using $b_k|h_\ell - h_j| \leq b_k a_k^{-2}|\mu_\ell - \mu_j| \leq a_k^{-2} b_k^{-m+1}$, it follows that

$$h_j^{1/2}\|(K_{h_\ell} - K_{h_j})\gamma u_j\|_{L^2} = \mathbb{O}(b_k^{-m}), \quad j, \ell \in I_k,$$

if k is sufficiently large. The assumptions on w_j imply $\|w_j - u_j\|_{H^1} = \mathbb{O}(h_j^{1+\dim X})$. Here we use the estimate $\|v\|_{H^1}^2 \leq C\|v\|_{L^2}\|v\|_{H^2}$. Applying the trace theorem, $\|\gamma w_j - \gamma u_j\|_{L^2} = \mathbb{O}(h_j^{1+\dim X})$. Summarizing the estimates, we have shown that, for some $\varepsilon > 0$,

$$\|h_j^{1/2} K_{h_\ell}\gamma w_j - f_j\|_{L^2} = \mathbb{O}(h_\ell^{\varepsilon+\dim X}), \quad j, \ell \in I_k.$$

Because of almost orthogonality of the f_j and the Weyl estimate, we can apply [Stefanov 1999, Lemma 4]. We obtain, for every $\ell \in I_k$, the linear independence of $\{K_{h_\ell}\gamma w_j\}_{j \in I_k}$ when k is sufficiently large. Since $K_{h_\ell}\gamma$ is linear, also $\{w_j\}_{j \in I_k}$ is linearly independent. ◻

Proof of Corollary 2. We apply Proposition 21 with $\mu_j \uparrow \infty$ the sequence of positive eigenvalues of P, counted with multiplicities, and $\{f_j\}$ a corresponding orthonormal system of eigenvectors. Fix $m > \dim X$. Let $[a_k, b_k]$ be the intervals, clustering $\{\mu_j\}$, given in the proposition. The quasimode states defined in (52) belong to the domain of the selfadjoint operator L_T. Let π_k denote the spectral projector for L_T of the interval $[a'_k, b'_k]$, where $a'_k = a_k - \delta b_k^{-m-\dim X}$, $b'_k = b_k + \delta b_k^{-m-\dim X}$. The intervals $[a'_k, b'_k]$ are pairwise disjoint. Set $w_j = \pi_k u_j$ if $\mu_j \in [a_k, b_k]$. A well-known argument, using the spectral theorem, gives

$$\delta^2 b_k^{-2m-2\dim X} \|w_j - u_j\|_{L^2}^2 \le \|(L_T - \mu_j^2)u_j\|_{L^2}^2 = \mathbb{O}(b_k^{-\infty})$$

if $\mu_j \in [a_k, b_k]$. Since L_T is elliptic, we have $\|w_j\|_{H^2} = \mathbb{O}(\mu_j^2)$. Now Proposition 21, with $N = 0$, implies that, for k sufficiently large, the rank of π_k equals $\sharp\{j\ ;\ \mu_j \in [a_k, b_k]\}$. Hence an increase by n of N_P over $[a_k, b_k]$ leads to an increase $\ge n$ of N_{L_T} over $[a'_k, b'_k]$. Taking into account the widths of the intervals, the corollary follows. □

Remark. The foregoing arguments also apply to give lower bounds for the counting function of resonances. In this case, π_k is the projector onto the space of resonant states which correspond to resonances in rectangles $[a_k, b_k] + i[0, s_k]$. To satisfy the assumptions in Proposition 21 for $w_j = \pi_k u_j$, one establishes resolvent estimates. See [Stefanov and Vodev 1996; Tang and Zworski 1998; Stefanov 1999; Stefanov 2000] for ways from quasimodes to resonances. The clustering method was developed in this context [Stefanov 1999] to handle multiplicities appropriately. Resolvent estimates for anisotropic elastic systems are given in [Kawashita and Nakamura 2000].

10. The isotropic subprincipal symbol

In this section we assume that the elastic medium is isotropic. We evaluate the subprincipal symbol of P, p_{sub}, starting from the general formula (50).

We continue with Example 8, referring to the notation introduced there. The kernel bundle $\ker z$ is a line subbundle of V, the subbundle of $\mathbb{C}T_X M$ spanned by ν, $\hat{\xi} = \xi/|\xi|$. Abbreviate (19) and (18) as follows:

$$(z)_{11} = \begin{bmatrix} \zeta_1 & -i\zeta_2 \\ i\zeta_2 & \zeta_3 \end{bmatrix}, \quad (iq)_{11} = \begin{bmatrix} \kappa_{11} & -i\kappa_{12} \\ i\kappa_{21} & \kappa_{22} \end{bmatrix}.$$

It will be convenient to use the velocities relative to the Rayleigh wave speed, $\sigma_s = c_r/c_s$ and $\sigma_p = c_r/c_p$. Then $t = \sigma_s^2$, $ut = \sigma_p^2$ on $\Sigma = \{c_r|\xi| = 1\}$. Moreover, we set $\tau_s = (1-\sigma_s^2)^{1/2}$, $\tau_p = (1-\sigma_p^2)^{1/2}$,

We first show how to evaluate $(z_- v \mid v)$, $v \in \ker z$, z_- as in (45).

Lemma 22. *Set $K = (iq)_{11}$. Define Y_j by* (55), (56), *and* (58) *below. Let $X = (x_{jk})$ the selfadjoint 2×2 matrix which is the unique solution of*

$$XK + K^* X = -2Y_1 - Y_2 - Y_2^* + Y_3 + Y_3^*. \tag{54}$$

Let $v = v_1 \nu + v_2 \hat{\xi} \in \ker z$. Then

$$2\,\mathrm{Re}(z_- v \mid v) = x_{11}|v_1|^2 + x_{22}|v_2|^2 + 2\,\mathrm{Re}\, x_{12}\bar{v_1} v_2.$$

Proof. Set $x = z_- + z_-^*$. Then $2\,\mathrm{Re}(z_- v \mid v) = (xv \mid v)$. By (45), x satisfies the uniquely solvable Sylvester equation $x(iq) + (iq)^* x = iy + (iy)^*$, where y equals the right-hand side of (45). Since q

leaves V and $V^\perp$ invariant, $X=(x)_{11}=(x_{jk})$ is the unique solution of (54) provided the right-hand side of the equation equals $(iy+(iy)^*)_{11}$. The latter holds if

$$Y_1=(\operatorname{tr}(S)z+\partial_r z)_{11},\quad Y_2=(a_{1-}iq)_{11},\quad Y_3=\big(i\operatorname{tr}{}^v\nabla(iq)^*.a\,{}^h\nabla iq\big)_{11}.$$

Observe that the a_{2-} term of (45) drops out because of the skewness of $(ia_{2-})_{11}$. In the following we derive formulas for Y_j.

The basis vectors ν and $\hat{\xi}$ do not depend on r. Therefore, $(\partial_r z)_{11}=\partial_r(z)_{11}$. We obtain

$$Y_1=\operatorname{tr}(S)\begin{bmatrix}\zeta_1 & -i\zeta_2\\ i\zeta_2 & \zeta_3\end{bmatrix}+\begin{bmatrix}\partial_r\zeta_1 & -i\partial_r\zeta_2\\ i\partial_r\zeta_2 & \partial_r\zeta_3\end{bmatrix}. \tag{55}$$

Using Lemma 12 and the remark following it we obtain a formula for $(a_{1-})_{11}$. Clearly, $(a_{1-}iq)_{11}=(a_{1-})_{11}(iq)_{11}$. We derive

$$Y_2=\begin{bmatrix}\mu\operatorname{tr}S & \langle\hat{\xi},\nabla\mu\rangle\\ \langle\hat{\xi},\nabla\lambda\rangle & \mu\operatorname{tr}S+(\lambda+\mu)\langle\hat{\xi},S\hat{\xi}\rangle\end{bmatrix}\begin{bmatrix}\kappa_{11} & -i\kappa_{12}\\ i\kappa_{21} & \kappa_{22}\end{bmatrix}. \tag{56}$$

It remains to determine Y_3. Fix an orthonormal frame (η_j) of $T^*_X M$, $\eta_1=\nu$, $\eta_2=\hat{\xi}$. To compute the contraction we use the frame $(\eta_j)_{j\geq 2}$ of T^*X, and the dual frame. We compute derivatives of

$$iq=|\xi|\sqrt{1-t}(\operatorname{Id}-\nu\otimes\nu-\hat{\xi}\otimes\hat{\xi})\qquad+\kappa_{11}\nu\otimes\nu-i\kappa_{12}\nu\otimes\hat{\xi}+i\kappa_{21}\hat{\xi}\otimes\nu+\kappa_{22}\hat{\xi}\otimes\hat{\xi}.$$

Set $s_{jk}=\langle S\eta_j,\eta_k\rangle$. A calculation using ${}^h\nabla\nu=S$ and ${}^h\nabla\hat{\xi}=0$ gives

$$\big({}^h\nabla_j iq\big)_{11}={}^h\nabla_j(iq)_{11}+s_{j2}|\xi|b^{-1}M,\quad j\geq 2,$$

where

$$M=\begin{bmatrix}0 & (ut-b)\sqrt{1-t}\\ (ut-b)\sqrt{1-t} & i(ut-t)\end{bmatrix}.$$

Regard the coefficients κ_{jk} as functions of $c_s, c_p, |\xi|$. Then ${}^h\nabla_j(iq)_{11}=\langle\eta_j,\nabla c_s\rangle K_s+\langle\eta_j,\nabla c_p\rangle K_p$, where K_s and K_p denote the partial derivatives of $(iq)_{11}$ with respect to c_s and c_p, respectively. In particular,

$$\big({}^h\nabla_2 iq\big)_{11}=\langle\hat{\xi},\nabla c_s\rangle K_s+\langle\hat{\xi},\nabla c_p\rangle K_p+s_{22}|\xi|b^{-1}M.$$

Define $w_1=[(ut-b)\sqrt{1-t},-i(b-ut)]$. The row $k>2$ in $\big({}^h\nabla_j iq\big)_{21}$ equals $s_{jk}b^{-1}|\xi|w_1$.

The vertical derivative of a function κ which, when restricted to a fiber depends only on $|\xi|$, is given by its radial derivative:

$${}^v\nabla_\eta\kappa=|\xi|^{-1}\langle\hat{\xi},\eta\rangle\dot{\kappa}. \tag{57}$$

A calculation using ${}^v\nabla\nu=0$ and ${}^v\nabla\hat{\xi}=|\xi|^{-1}(\operatorname{Id}-\hat{\xi}\otimes\hat{\xi})$ gives

$$\big({}^v\nabla_j iq\big)_{11}={}^v\nabla_j(iq)_{11}=|\xi|^{-1}\delta_{2j}\dot{K},\quad j\geq 2,$$

where we have set

$$\dot{K}=\begin{bmatrix}\dot{\kappa_{11}} & -i\dot{\kappa_{12}}\\ i\dot{\kappa_{21}} & \dot{\kappa_{22}}\end{bmatrix}.$$

Define $w_2=[i(b-t),\sqrt{1-ut}-\sqrt{1-t}]$. The row $k>2$ in $\big({}^v\nabla_j iq\big)_{21}$ equals $\delta_{jk}b^{-1}w_2$.

Set $A = (a)_{11} = \operatorname{diag}[\lambda + 2\mu, \mu]$. Note that $(a)_{22}$ equals μ times the unit matrix. Summing over $j \geq 2$ we derive

$$Y_3 = i\dot{K}^* A\big(|\hat{\xi}|^{-1}\langle\hat{\xi}, \nabla c_s\rangle K_s + |\hat{\xi}|^{-1}\langle\hat{\xi}, \nabla c_p\rangle K_p + s_{22}b^{-1}M\big) + i\mu b^{-2}|\xi|(\operatorname{tr}(S) - s_{22})w_2^* \otimes w_1, \quad (58)$$

evaluated at Σ. □

Denote by v the unique unit section of $\ker(z - \lambda_0)$ satisfying $(\hat{\xi} \mid v) > 0$, so

$$v = \gamma^{-1}\big(i\zeta_2 \nu + (\zeta_1 - \lambda_0)\hat{\xi}\big),$$

$\gamma > 0$ such that $|v| = 1$. We compute the v-dependent terms in the right-hand side of (50).

Lemma 23. *On* Σ *we have* $\operatorname{Im}\operatorname{tr} {}^h\nabla p.{}^v\nabla v^*.v = 0$, *and*

$$16\gamma^2 \operatorname{Im}\operatorname{tr}(v^* {}^v\nabla z.{}^h\nabla v)$$
$$= m^3\mu^{-1}c_r^2\sigma_s^6(4-\sigma_s^2)(2-\sigma_s^2)\big(2\tau_s\dot{\zeta}_3 - (2-\sigma_s^2)\dot{\zeta}_2\big)s_{22} + 2m^3c_r\sigma_s^6(2-\sigma_s^2)(5\sigma_s^2 - 4 - \sigma_s^4)\operatorname{tr}' S, \quad (59)$$

where $\operatorname{tr}' S = \operatorname{tr} S - s_{22}$, $s_{22} = \langle\hat{\xi}, S\hat{\xi}\rangle$, *and* $m = \mu|\xi|/b$.

Proof. Set $\gamma_1 = \zeta_2/\gamma$ and $\gamma_2 = (\zeta_1 - \lambda_0)/\gamma$. We continue to use the frame (η_j). For $j \geq 2$ we have

$$ {}^v\nabla_j v^* = -i\,{}^v\nabla_j\gamma_1.\nu^* + {}^v\nabla_j\gamma_2.\hat{\xi}^* + |\xi|^{-1}(1 - \delta_{2j})\gamma_2\eta_j^*,$$
$$ {}^h\nabla_j v = i\,{}^h\nabla_j\gamma_1.\nu + {}^h\nabla_j\gamma_2.\hat{\xi} + i\gamma_1 S\eta_j.$$

Note that ${}^v\nabla_j v^*.v$ is real. Hence $\operatorname{Im}\operatorname{tr} {}^h\nabla p.{}^v\nabla v^*.v = 0$. We need the vertical derivative of z. To compute it we proceed in the same way as we did when computing the derivatives of iq. Recall that z equals $\zeta^\perp \operatorname{Id}$ on $V^\perp$, where $\zeta^\perp = \mu|\xi|\sqrt{1-t}$. We obtain $\big({}^v\nabla_j z\big)_{11} = {}^v\nabla_j(z)_{11}$. Moreover, the column $k > 2$ in $({}^v\nabla_j z)_{12}$ equals $\delta_{jk}|\xi|^{-1}$ times the transpose of the row vector $[-i\zeta_2, \zeta_3 - \zeta^\perp]$. We get

$$\operatorname{Im} v^* {}^v\nabla_j z.{}^h\nabla_j v = \gamma_1 \operatorname{Re} v^* {}^v\nabla_j z.S\eta_j$$
$$= \gamma_1(\gamma_2 {}^v\nabla_j\zeta_3 - \gamma_1 {}^v\nabla_j\zeta_2)s_{2j} + \gamma_1|\xi|^{-1}\big(\gamma_2(\zeta_3 - \zeta^\perp) - \gamma_1\zeta_2\big)s_{jj}(1 - \delta_{2j}).$$

Summing over $j \geq 2$ we obtain

$$\gamma^2 \operatorname{Im}\operatorname{tr}(v^* {}^v\nabla z.{}^h\nabla v) = \zeta_1\zeta_2 {}^v\nabla_{S\hat{\xi}}\zeta_3 - \zeta_2^2 {}^v\nabla_{S\hat{\xi}}\zeta_2 + c_r\zeta_2\big(\zeta_1(\zeta_3 - \zeta^\perp) - \zeta_2^2\big)\operatorname{tr}'(S).$$

The first term on the right equals

$$m^2|\xi|^{-1}s_{22}(2b - t)\big(t\sqrt{1-t}\,\dot{\zeta}_3 - (2b - t)\dot{\zeta}_2\big).$$

Moreover, using the definition of b, we calculate

$$\zeta_3 - \zeta^\perp = m(\sqrt{1 - ut} - \sqrt{1 - t}).$$

Using (21), $4b = t(4 - t)$, we derive (59). □

The restriction to Σ of the radial derivative of the eigenvalue $\lambda_0 = (zv \mid v) = a_0^{-2}(p - 1)$ equals $\dot{\lambda}_0 = (\dot{z}v \mid v) = a_0^{-2}$ because $\dot{p} = 1$ on Σ.

Lemma 24. *Let $m = \mu|\xi|/b$. On Σ, we have*

$$\gamma^2 \dot{\lambda}_0 = m^3 \sigma_s^6 (4-\sigma_s^2)\tau_s \bigl(\tau_p/\tau_s + c_s\tau_s/c_p\tau_p + \sigma_s^2 - 2\bigr),$$

Proof. The section $w = i\zeta_2 \nu + \zeta_1 \hat{\xi}$ equals γv on Σ. Therefore $\gamma^2\lambda_0 \equiv (zw \mid w) = \zeta_1 \det(z)_{11}$ to second order on Σ. Inserting (20),

$$\gamma^2\lambda_0 \equiv mbt\sqrt{1-t}\bigl(4\sqrt{(1-t)(1-ut)} - (2-t)^2\bigr).$$

Recall that $p = c_r|\xi| = \sigma_s t^{-1/2}$, $\Sigma = \{t = \sigma_s^2\}$. The rule of de l'Hospital gives

$$\lim_{t\to\sigma_s^2} \frac{4\sqrt{(1-t)(1-ut)} - (2-t)^2}{\sigma_s t^{-1/2} - 1} = 4\sigma_s^2\bigl(\tau_p/\tau_s + c_s\tau_s/c_p\tau_p + \sigma_s^2 - 2\bigr).$$

Summarizing, the formula for $\gamma^2\dot{\lambda}_0 = \gamma^2\lambda_0/(p-1)$ follows. □

Inserting the formulas of the lemmas of this section into the general formula (50) for the subprincipal symbol of P we obtain a formula for the subprincipal symbol in the isotropic case.

Proposition 25. *Denote by $X = (x_{jk})$ the 2×2 matrix solving* (54). *Set*

$$N = \tau_s\bigl(\tau_p/\tau_s + c_s\tau_s/c_p\tau_p + \sigma_s^2 - 2\bigr).$$

Let P be the operator of Lemma 20 determined by the unit section v of ker *z having positive $\hat{\xi}$ component. The subprincipal symbol of P is given as follows.*

$$\begin{aligned}16Np_{\mathrm{sub}} &= (c_r/2\mu)\bigl(x_{11}(2-\sigma_s^2)^2 + 4x_{22}(1-\sigma_s^2)^2 + 4\,\mathrm{Im}\,x_{12}(2-\sigma_s^2)\tau_s\bigr)\\ &\quad + \mu^{-1}c_r^2(2-\sigma_s^2)\bigl(2\tau_s\dot{\zeta}_3 - (2-\sigma_s^2)\dot{\zeta}_2\bigr)\langle S\hat{\xi},\hat{\xi}\rangle + 2c_r(4-\sigma_s^2)^{-1}(2-\sigma_s^2)(5\sigma_s^2 - 4 - \sigma_s^4)(\mathrm{tr}(S) - \langle S\hat{\xi},\hat{\xi}\rangle).\end{aligned}$$

Proof. On Σ, $w = \gamma v = (mt/2)\bigl(i(2-t)\nu + 2\sqrt{1-t}\hat{\xi}\bigr)$. Using Lemmas 22 and 24 we calculate $16N\,\mathrm{Re}(z_{-}w \mid w)/\gamma^2\dot{\lambda}_0$. The result is the first term on the right-hand side of the claimed formula. Similarly, we obtain the other terms combining the Lemmas 23 and 24. □

The constituents of the above formula for p_{sub} are curvature and velocities (Lamé parameters), assumed known. It seems difficult to analyze the formula further unless it is specialized to particular cases. However, it should be noted that the formula allows explicit numerical evaluation of p_{sub}. Therefore it can be used when solving transport equations for Rayleigh wave amplitudes numerically with a (seismic) ray tracing program, say. Formulas for the amplitudes of Rayleigh waves were given by in [Babich and Kirpichnikova 2004].

Appendix: Geometric pseudodifferential calculus

Pseudodifferential operators on manifolds are usually introduced by reducing to the euclidean case via partitions of unity, [Hörmander 1985, 18.1; Zworski 2011]. The principal symbol of a pseudodifferential operator is invariantly defined. If the operator acts on sections of the line bundle of half-densities then there also is an invariantly defined subprincipal symbol [Hörmander 1985, Theorem 18.1.33; Sjöstrand and Zworski 2002, Appendix].

In the body of the paper we explicitly track, down to the subprincipal level, symbols of operators acting between vector bundles. To achieve this we use Sharafutdinov's geometric pseudodifferential calculus [Sharafutdinov 2004; 2005]. The purpose of this appendix is to recall this calculus, presenting a semiclassical variant. Since we have to refer, in the main part of the present paper, to proofs of the calculus, we give a rather detailed presentation. The calculus depends on a symmetric connection of the manifold and on metric connections of the (Hermitian) bundles. We make the stronger assumption that the manifold is Riemannian and that the symmetric connection is the Levi-Civita connection. The important features of the calculus are a symbol isomorphism modulo order minus infinity, and complete symbol expansions for products and adjoints given solely in terms of geometric data. Using connections to develop a pseudodifferential calculus and to prove the existence of a complete symbol isomorphism was done earlier in [Widom 1980]. This was further developed by Pflaum [1998], who gave a convenient quantization map from symbols to operators. Sharafutdinov gave symbol expansions in terms of geometric data.

Let X a compact Riemannian manifold without boundary, $\dim X = n$. The exponential map, exp, of the Levi-Civita connection defines a diffeomorphism, $(x, v) \mapsto (x, y) = (x, \exp_x v)$, between a neighborhood of the zero-section of the tangent bundle $T = TX$ and a neighborhood of the diagonal in X^2. In the proofs of the propositions below we need the following properties of exp. In local coordinates the exponential map satisfies

$$(\exp_x v)^i = x^i + v^i - \Gamma^i_{jk}(x) v^j v^k/2 + \mathcal{O}(|v|^3), \tag{60}$$

where Γ^i_{jk} denotes the Christoffel symbols. Normal coordinates centered at x satisfy $(\exp_x v)^i = v^i$. There exist $0 < r < R < \operatorname{inj}(x)$, the injectivity radius of X, such that the equation

$$\exp_{\exp_x v} z = \exp_x w \tag{61}$$

defines, for every $v \in T_x = T_x X$, $|v| < R$, a diffeomorphism $w \mapsto z = z(x, v, w)$ from an open neighborhood of the origin, contained in $\{|w| < R\} \subset T_x$, onto the ball $\{|z| < r\} \subset T_y$, $y = \exp_x v$. This map is used below to change variables of integration. Obviously, $z(x, 0, w) = w$. A computation in normal coordinates centered at x shows that

$$(z'_w)^{-1} z = w - v + \mathcal{O}((|v| + |w|)^3) \quad \text{as } v, w \to 0. \tag{62}$$

Recall, from Section 3, the notation for segments and for parallel transport maps. In local coordinates,

$$\big(\tau^{TX}_{[\exp_x v \leftarrow x]} w\big)^i = w^i - \Gamma^i_{jk}(x) w^j v^k + \mathcal{O}(|v|^2). \tag{63}$$

Let $E \to X$ and $F \to X$ be Hermitian vector bundles with metric connections. Recall from Section 3 the definition (24) of horizontal derivatives and the definition of vertical derivatives. A C^∞ section a of the bundle $\pi^* \operatorname{Hom}(E, F) \to T^* X$ is called a $\operatorname{Hom}(E, F)$-valued symbol of order $m \in \mathbb{R}$, $a \in S^m = S^m(T^* X; \pi^* \operatorname{Hom}(E, F))$, if and only if for all nonnegative integers j and ℓ,

$$\sup_{x,\xi} (1 + |\xi|)^{j-m} \big|({}^v\nabla)^j ({}^h\nabla)^\ell a(x, \xi)\big| < \infty.$$

These are the usual type $(1, 0)$ symbol estimates. The symbol space S^m is a Fréchet space. The space $S^{m,k} = S^{m,k}(T^* X; \pi^* \operatorname{Hom}(E, F))$ of h-dependent symbols of order m and degree k is the Fréchet space of families $a_h \in S^m$ such that $\{h^k a_h\,;\, 0 < h \le 1\}$ is bounded in S^m. We call $a \in S^{m,k}$ classical if there exists an asymptotic expansion $a \sim \sum_j h^{j-k} a_j$ with h-independent symbols $a_j \in S^{m-j}$.

In the following lemma we define, in a semiclassical setting, the quantization of symbols according to Sharafutdinov's geometric pseudodifferential calculus. We relate this definition of h-pseudodifferential operators to the definition in the euclidean situation. For semiclassical analysis, in particular, for the class $\Psi^{m,k} = \mathrm{Op}_h\, S^{m,k}$ of h-pseudodifferential operators, including mapping properties, and for frequency sets (h-wavefront sets), refer to [Gérard 1988; Ivrii 1998; Dimassi and Sjöstrand 1999; Sjöstrand and Zworski 2002; Zworski 2011]. The class of negligible operators, $\Psi^{-\infty,-\infty}$, consists of h-dependent operators whose Schwartz kernels are C^∞ with $\mathbb{O}(h^\infty)$ seminorms.

Fix $\chi_0 \in C^\infty(TX)$, real-valued, $|v| < r$ on the support of $\chi_0(x, v)$, such that $\chi_0 = 1$ in a neighborhood of the zero-section in TX.

Lemma 26. *Let $a_h \in S^{m,k}$ be a* Hom(E, F)*-valued symbol. Then*

$$A_h u_h(x) = (2\pi h)^{-n} \int_{T_x^*} \int_{T_x} e^{-i\langle \eta, v\rangle/h} \chi_0(x, v) \cdot a_h(x, \eta) \tau^E_{[x \leftarrow \exp_x v]} u_h(\exp_x v)\, \mathrm{d}v\, \mathrm{d}\eta, \tag{64}$$

defines an h-pseudodifferential operator $A_h \in \Psi^{m,k}(X; E, F)$. Given a point x there exists a geodesic ball U centered at x, and a symbol $a_h^U \in S^{m,k}$ such that, for u_h compactly supported in U,

$$A_h u_h(y) = (2\pi h)^{-n} \int_{T_x^*} \int_{T_x} e^{i\langle \theta, v-w\rangle/h} a_h^U(y, \theta) \tau^E_{[y \leftarrow y']} u_h(y')\, \mathrm{d}w\, \mathrm{d}\theta,$$

where $y = \exp_x v$ and $y' = \exp_x w$. Moreover, at x, $a_h^U \equiv a_h$ modulo $S^{m-2,k-2}$. Every h-pseudodifferential operator is, modulo negligible operators, of the form (64).

The measures in (64) are the normalized Lebesgue measures of the euclidean spaces T_x and T_x^*.

Proof. We shall drop the subscript h from the notation. Fix $x \in X$. Let U denote a geodesic ball with center x and radius $\le R$. In the following we assume that the support of u is a compact subset of U. In (64) we replace the variables x, v, η by y, z, ζ. Next we change variables in the integral $Au(y)$ such that the domain of integration does not depend on y. Set $y = \exp_x v$. Define $z = z(x, v, w)$ by (61). Using the symplectic map $(w, \vartheta) \mapsto (z, \zeta)$, $\zeta = {}^t(z'_w)^{-1}\vartheta$, we get

$$Au(y) = \int_{T_x} K(v, w) \tau^E_{[y \leftarrow \exp_x w]} u(\exp_x w)\, \mathrm{d}w,$$

where the kernel K is given by

$$K(v, w) = (2\pi h)^{-n} \int_{T_x^*} e^{-i\varphi/h} \chi_0(y, z) a(y, \zeta)\, \mathrm{d}\vartheta,$$

with $\varphi = \langle \zeta, z\rangle = \langle \vartheta, (z'_w)^{-1} z\rangle$. Since $z = 0$ if and only if $v = w$, we have $\varphi(v, w, \vartheta) = \langle \psi(v, w)\vartheta, w - v\rangle$. Here $\psi = \mathrm{Id} + \mathbb{O}(|v|^2 + |w|^2)$ by (62). Decreasing the radius of U and making the linear change of variables $\theta = \psi(v, w)\vartheta$, we get

$$K(v, w) = (2\pi h)^{-n} \int_{T_x^*} e^{i\langle \theta, v-w\rangle/h} \chi_0(y, z) a(y, \zeta) J_1(v, w)\, \mathrm{d}\theta,$$

with $J_1(v,w) = 1+\mathbb{O}(|v|^2+|w|^2)$. It follows that A restricted to U is an h-pseudodifferential operator of class $\Psi^{m,k}$. As it stands the symbol depends on v, θ, w. Using the standard symbol reduction procedure we obtain $a^U(\exp_x v, \theta)$. Moreover, the asymptotic expansion implies that, as $v \to 0$, $a^U - a \in S^{m-2,k-2}$.

Note that $Au(y) = 0$ if the distance between y and $\operatorname{supp} u$ is $> r$. Using a partition of unity, we infer that the class of operators given by (64) equals the class of h-pseudodifferential operators with Schwartz kernels supported in small neighborhoods of the diagonal. □

Standard arguments show that up to a negligible operator $A_h = \operatorname{Op}_h(a_h)$ does not depend on the choice of the cutoff χ_0. The space

$$\Psi^{m,k}(X; E, F) = \operatorname{Op}_h S^{m,k} + \Psi^{-\infty,-\infty}.$$

is the space h-pseudodifferential order m and degree k. We denote the geometric symbol by $\sigma_h(A_h) = a_h$.

Remark. Let $A_h = \operatorname{Op}_h(a_h) \in \Psi^{0,0}$. Then A_h is L^2 bounded, uniformly in h. Assume, in addition, that a_h depends differentiably on h with $\partial_h a_h \in S^{0,0}$. Changing variables in (64) from η to $\xi = \eta/h$, we obtain $A_{h_1} - A_{h_0} = \int_{h_0}^{h_1} h^{-1} \operatorname{Op}_h(b_h)\,\mathrm{d}h$, where $b_h \in S^{0,0}$, $b_h(x,\eta) = h\partial_h a_h(x,\eta) + {}^v\nabla_\eta a_h(x,\eta)$. This implies the following useful Lipschitz estimate:

$$\|A_{h_1} - A_{h_0}\|_{L^2\to L^2} \le C h_0^{-1}|h_1 - h_0| \quad \text{if } h_0 < h_1,$$

where $\|\operatorname{Op}_h(b_h)\|_{L^2\to L^2} \le C < \infty$. The assumption holds if a_h is classical and given as a Borel sum.

In the following, we often suppress from writing the h-dependence of symbols, operators and distributions. Moreover, when dealing with integrals like (64), we move, without explicitly writing this, the x-dependence from the domain of integration into the integrand using arguments as in the proof of the lemma.

Lebesgue measure $\mathrm{d}v$ on $T_x X$ and Riemannian volume are related by

$$\int f(y)\,\mathrm{d}V_X(y) = \int f(\exp_x v) J_0(x,v)\,\mathrm{d}v,$$

where $y = \exp_x v$ and J_0 is the Jacobian, satisfying $J_0 = 1+\mathbb{O}(|v|^2)$ at $v = 0$. Let $A = A_h$ be as in (64). The Schwartz kernel K_A of A,

$$Au(x) = \int_X K_A(x,y)u(y)\,\mathrm{d}V_X(y), \quad K_A(x,y) \in \operatorname{Hom}(E_y, F_x).$$

equals in a neighborhood of the diagonal a partial Fourier transform of the symbol,

$$K_A(x,y) = (2\pi h)^{-n} \int_{T_x^*} e^{-i\langle \eta, \exp_x^{-1} y\rangle/h} a(x,\eta)\,\mathrm{d}\eta\, \psi(x,y)\tau^E_{[x\leftarrow y]}. \tag{65}$$

Here $\psi(x,y) = \chi_0(x,v)/J_0(x,v)$, $y = \exp_x v$. The symbol a is recovered via the inverse Fourier transform:

$$a(x,\xi) \equiv \int_{T_x} e^{i\langle \xi, v\rangle/h} (\chi_0 J_0)(x,v) K_A(x, \exp_x v)\tau^E_{[\exp_x v\leftarrow x]}\,\mathrm{d}v \tag{66}$$

modulo $S^{-\infty,-\infty}$. The correspondence between an operator $A = \mathrm{Op}_h(a)$ and its full symbol a, named the geometric symbol of A, defines the complete symbol isomorphism

$$\Psi^{m,k}(X; E, F)/\Psi^{-\infty,-\infty} \cong S^{m,k}(T^*X; \mathrm{Hom}(\pi^*E, \pi^*F))/S^{-\infty,-\infty}.$$

The geometric symbol can also be computed by applying the operator to suitable testing functions:

$$a(x,\xi)s \equiv A_y\big(e^{i\langle \xi, \exp_x^{-1} y\rangle/h}\chi_0(x, \exp_x^{-1} y)\tau^E_{[y\leftarrow x]}s\big)|_{y=x}. \tag{67}$$

Here A_y means that A acts on functions of the variable y. In particular, in case $E = \mathbb{C}$, the geometric symbol is obtained at the center of normal coordinates x^j when A is applied to $e^{i\xi_j x^j/h}$ and evaluated at $x^j = 0$.

We derive symbol properties and expansions using the method of stationary phase:

$$\begin{aligned}\big(\det(H/2\pi i h)\big)^{1/2}\int e^{i(\varphi(x))/h}a(x)\,\mathrm{d}x &= \exp\big(2^{-1}ih\langle H^{-1}\partial,\partial\rangle\big)\big(e^{i\rho(x)/h}a(x)\big)\big|_{x=0}\\ &= \sum_{j<3N}\frac{(ih)^j}{j!2^j}\langle H^{-1}\partial,\partial\rangle^j\big(e^{i\rho(x)/h}a(x)\big)\big|_{x=0} + \mathbb{O}(h^N).\end{aligned}$$

Here $\varphi \in C^\infty$ is real-valued, $\varphi'(x) = 0$ if and only if $x = 0$, $H = \varphi''(0)$ is nonsingular, and $\varphi(0) = 0$. The remainder $\rho(x) = \varphi(x) - \langle Hx, x\rangle/2$ vanishes to third order at $x = 0$. The expansion has the advantage, when compared to that obtained using the Morse lemma, of giving an efficient algorithm for computing the asymptotic series.

See [Asada and Fujiwara 1978, Lemma 3.2] and [Hörmander 1990, Theorem 7.7.5], where the expansion is arranged in powers of $\omega^{-1} = h$.

We are mainly interested in the leading symbols of operators. We define the leading symbol of an operator $\mathrm{Op}_h(a) \in \Psi^{m,k}$ as the residue of a in $S^{m,k}/S^{m-2,k-2}$. The principal symbol is, of course, the residue in $S^{m,k}/S^{m-1,k-1}$.

Proposition 27. *Let $A = \mathrm{Op}_h(a)$ as in* (64) *with geometric symbol $a \in S^{m,k}$. The formal adjoint $A^* \in \Psi^{m,k}(X; F, E)$ has the geometric symbol*

$$b \equiv a^* - ih\,\mathrm{tr}\,{}^v\nabla\,{}^h\nabla a^* \quad \mathrm{mod}\ S^{m-2,k-2}. \tag{68}$$

If a is classical then so is b.

Notice that ${}^v\nabla\,{}^h\nabla a^*$ is a section of $\pi^*(\mathrm{Hom}(F, E)\otimes T\otimes T^*)$. The trace is taken of the $T\otimes T^*$ part.

Proof. The formal adjoint of A is defined by

$$\int_X \big(u_1(x) \mid Au_2(x)\big)_F\,\mathrm{d}V_X(x) = \int_X \big(A^*u_1(y) \mid u_2(y)\big)_E\,\mathrm{d}V_X(y).$$

The Schwartz kernel satisfies $K_{A^*}(x, y) = K_A(y, x)^*$. Recall that parallel transport preserves inner products. It follows from (65) that

$$K_{A^*}(x, y) = (2\pi h)^{-n}\int_{T_y^*} e^{i\langle \eta, \exp_y^{-1} x\rangle/h}\tau^E_{[x\leftarrow y]}a(y,\eta)^*\mathrm{d}\eta\,\psi(y, x),$$

and $K_{A^*}(x, y) = 0$ if the distance between x and y is $> r$. Set $y = \exp_x v$. Define $z \in T_y$ by $\exp_y z = x$. After a linear change variables from $\eta \in T_y^*$ to $\zeta = {}^t(\exp'_x(v))\eta \in T_x^*$ we have

$$K_{A^*}(x, y) = (2\pi h)^{-n} \int_{T_x^*} e^{i\langle \eta, z\rangle/h} \tau^E_{[x\leftarrow y]} a(y, \eta)^* \mathrm{d}\zeta \ \psi(y, x)/J_1(x, v),$$

with Jacobian $J_1(x, v) = 1 + \mathbb{O}(|v|^2)$. Define

$$b(x, \xi) = \int_{T_x} e^{i\langle \xi, v\rangle/h} (\chi_0 J_0)(x, v) K_{A^*}(x, y) \tau^F_{[y\leftarrow x]} \mathrm{d}v.$$

Inserting K_{A^*} we have

$$b(x, \xi) = (2\pi h)^{-n} \int_{T_x} \int_{T_x^*} e^{i\varphi/h} \tilde{a} J \,\mathrm{d}\zeta \,\mathrm{d}v, \tag{69}$$

where

$$\begin{aligned}
\varphi &= \langle \xi, v\rangle + \langle \eta, z\rangle = -\langle \zeta - \xi, v\rangle + \langle \zeta, \Phi\rangle, \\
\tilde{a} &= \tau^E_{[x\leftarrow y]} a(y, \eta)^* \tau^F_{[y\leftarrow x]} = \tau^{\mathrm{Hom}(F,E)}_{[x\leftarrow y]} a(y, \eta)^*, \\
J &= \chi_0(x, v) J_0(x, v) \psi(y, x)/J_1(x, v) = 1 + \mathbb{O}(|v|^2),
\end{aligned}$$

and $\Phi = \Phi(x, v) = \exp'_x(v)^{-1} z + v$. A computation in normal coordinates centered at x shows that $\Phi = \mathbb{O}(|v|^3)$ as $v \to 0$. If $\varphi'_\zeta = 0$ then $z = 0$, hence $v = 0$. It follows that the critical points of φ are defined by $v = 0$, $\zeta = \xi$.

Apply the method of stationary phase to (69) and deduce that $b \in S^{m,k}$. Moreover, the following asymptotic expansion holds:

$$b \sim \sum_j \frac{(ih)^j}{j!} \langle -\partial_\zeta, \partial_v\rangle^j \left(e^{i\langle \zeta, \Phi\rangle/h} \tilde{a}\right)\big|_{v=0,\zeta=\xi}. \tag{70}$$

Differentiation of the exponential factor brings out a nonzero factor only if it consumes at least three derivatives with respect to v and at most one derivative with respect to ζ. It follows that the sum is asymptotic. Moreover, b is determined modulo $S^{m-2,k-2}$ by the terms in the asymptotic sum with $j < 2$, $b \equiv a^* - ih\langle \partial_\zeta, \partial_v\rangle \tilde{a}$. Observe that

$$\tau^T_{[x\leftarrow \exp_x v]} \circ \exp'_x(v) = \mathrm{Id}_{T_x} + \mathbb{O}(|v|^2) \quad \text{as } v \to 0.$$

It follows that $\partial_v \tilde{a}\big|_{v=0} = {}^h\nabla a^*(x, \zeta)$. Hence $b \equiv a^* - ih \operatorname{tr} {}^v\nabla\, {}^h\nabla a^*$. The Schwartz kernels of $\mathrm{Op}_h(b)$ and A^* are equal in a neighborhood of the diagonal. Therefore $A^* - B \in \Psi^{-\infty,-\infty}$. ☐

Proposition 28. *Let $A \in \Psi^{m_A,k_A}(X; F, G)$ and $B \in \Psi^{m_B,k_B}(X; E, F)$ with geometric symbols a and b, respectively. Set $k = k_A + k_B$, $m = m_A + m_B$. Then $AB \in \Psi^{m,k}(X; E, G)$ with geometric symbol*

$$c \equiv ab - ih \operatorname{tr}\left({}^v\nabla a.{}^h\nabla b\right) \tag{71}$$

modulo $S^{m-2,k-2}$. If a and b are classical then so is c.

Again the trace is taken of the $T \otimes T^*$ part, and the dot terminates differentiated expressions.

Proof. Setting $y = \exp_x v$, the operator $C = AB$ is given by

$$Cu(x) = (2\pi h)^{-2n} \iiiint\limits_{T_x \times T_x^* \times T_y \times T_y^*} e^{-i(\langle \eta, v\rangle + \langle \zeta, z\rangle)/h} a(x,\eta) \cdot \tau^F_{[x\leftarrow y]}\big(b(y,\zeta)\tau^E_{[y\leftarrow \exp_y z]} u(\exp_y z)\big)\,\mathrm{d}z\,\mathrm{d}\zeta\,\mathrm{d}v\,\mathrm{d}\eta.$$

Here and in the following we do not write the cutoff factors. Let $z = z(x, v, w)$ be the solution of $\exp_y z = \exp_x w$. The symplectic change of variables $(w, \vartheta) \mapsto (z, \zeta)$, $\zeta = {}^t(z'_w)^{-1}\vartheta$, preserves the volume form. We get $Cu(x) = \int_{T_x} K_C(x, \exp_x w) u(\exp_x w) J_0(x, w)\,\mathrm{d}w$, with Schwartz kernel

$$K_C(x, \exp_x w) J_0(x, w) = (2\pi h)^{-2n} \int\limits_{T_x^* \times T_x \times T_x^*} e^{-i(\langle \eta, v\rangle + \langle \zeta, z\rangle)/h} c_0 \mathrm{d}(\vartheta, v, \eta)\, \tau^E_{[x\leftarrow \exp_x w]},$$

$c_0 = a(x,\eta)\tau^{\mathrm{Hom}(E,F)}_{[x\leftarrow y]} b(y,\zeta) M(x, w, v)$. Here $M(x, w, v) \in GL(E_x)$ denotes the parallel transport in E along the geodesic triangle $x \to \exp_x w \to \exp_x v \to x$. It follows that the symbol of C equals

$$c(x,\xi) = (2\pi h)^{-2n} \int\limits_{T_x \times T_x^* \times T_x \times T_x^*} e^{i\varphi/h} c_0 \mathrm{d}(v, \eta, w, \vartheta), \tag{72}$$

$\varphi = \langle \xi, w\rangle - \langle \eta, v\rangle - \langle \zeta, z\rangle$. We introduce $w - v$ as a new variable, w. Then (72) holds with

$$\varphi = -\langle \eta - \xi, v\rangle - \langle \vartheta - \xi, w\rangle + \langle \vartheta, \Phi\rangle,$$
$$c_0 = a(x,\eta)\tau^{\mathrm{Hom}(E,F)}_{[x\leftarrow y]} b(y,\zeta) M(x, w + v, v),$$

Here $\Phi = w - (z'_w(x, v, w + v))^{-1} z(x, v, w + v) \in T_x^*$. By (62), Φ vanishes to third order at $v = w = 0$. Clearly, $v = 0 = z$ at a critical point of φ. It follows that $v = w = 0$ and $\eta = \vartheta = \xi$ define the critical points.

Now apply the method of stationary phase to (72) and deduce that $c \in S^{m,k}$ is a symbol which, moreover, has an asymptotic expansion

$$c \sim \sum_j \frac{(-ih)^j}{j!} \big(\langle \partial_\vartheta, \partial_w\rangle + \langle \partial_\eta, \partial_v\rangle\big)^j \big(e^{i\langle \vartheta, \Phi\rangle/h} c_0\big)\big|_{v=w=0,\eta=\vartheta=\xi}. \tag{73}$$

Using that Φ does not depend on η and ϑ, and vanishes to third order at $v = w = 0$, we infer that the summands with $j > 1$ belong to $S^{m-2,k-2}$. It follows that

$$ab - ih\langle \partial_\eta a, \partial_v \tilde{b} M\rangle - iha\langle \partial_\vartheta, \partial_w\rangle \tilde{b} M,$$

evaluated at the critical point, is the leading symbol of C. Here $\tilde{b} = \tau^{\mathrm{Hom}(E,F)}_{[x\leftarrow y]} b(y,\zeta)$. We have $\partial_w \tilde{b} = 0$ at $v = w = 0$. This follows from $\zeta'_w = 0$ which is a corollary of $z = w$ at $v = 0$. The derivatives of M with respect to v and w vanish at $v = w = 0$. Using $\tau^T_{[x\leftarrow \exp_x v]} \circ z'_w = \mathrm{Id}_{T_x} + \mathcal{O}(|v|^2)$ at $w = 0$, we derive

$$\partial_v \tilde{b} = \partial_v \tau^{\mathrm{Hom}(E,F)}_{[x\leftarrow \exp_x v]} b(\exp_x v, {}^t(z'_w)^{-1}\vartheta) = {}^h\nabla b(x, \vartheta),$$

at $v = w = 0$. Summarizing the computations, (71) follows. □

Remark. The proofs of Propositions 27 and 28 follow those in [Sharafutdinov 2004; 2005] closely with only minor modifications. Our derivation of the asymptotic expansions of the symbols of adjoints and products may be somewhat shorter, however. We differ in defining the adjoint with respect to the volume element rather than using half-densities. Notice that the symbol expansions (70) and (73) depend only on the given symbols and on the geometry. In the formulas (68) and (71), we extracted the leading symbols.

For the purposes of the present paper it suffices to assume X compact. A symbol calculus on general (complete) Riemannian manifolds needs to take the injectivity radius into account and handle mapping properties more explicitly.

It is well-known that a pseudodifferential operator acting on half-densities has an invariantly defined subprincipal symbol; see [Sjöstrand and Zworski 2002, Appendix] for a proof in the semiclassical case. We relate the subprincipal symbol to the leading geometric symbol. Equip the half-density bundle $\Omega^{1/2} \to X$ with the inner product $(u \mid v) = u \cdot \bar{v} / \,\mathrm{d}V_X$, where the operations on the right are in the sense of densities. The connection given by $\nabla^{\Omega^{1/2}} \mathrm{d}V_X^{1/2} = 0$ is metric with respect to the Hermitian structure of $\Omega^{1/2}$.

Corollary 29. *Let $A \in \Psi^{m,k}(X; \Omega^{1/2})$. The leading symbol of A equals that of the corresponding scalar operator $\tilde{A} \in \Psi^{m,k}(X)$ which is given by $\tilde{A}u = \mathrm{d}V_X^{-1/2} A(u \,\mathrm{d}V_X^{1/2})$. If the geometric symbol a of A is classical, $a \sim \sum_{j\geq 0} h^{j-k} a_j$, $a_j \in S^{m-j}$, then $h^{-k} a_0$ is the principal symbol of A, and*

$$a_{\mathrm{sub}} = h^{1-k}(a_1 + i\, {}^{v}\nabla a_0 . {}^{h}\nabla a_0 / 2)$$

is its subprincipal symbol.

Proof. Consider the multiplication operator $\mathrm{d}V_X^{1/2} \in \Psi^{0,0}(X; \mathbb{C}, \Omega^{1/2})$. The $\mathrm{Hom}(\mathbb{C}, \Omega^{1/2})$-valued symbol $\pi^* \mathrm{d}V_X^{1/2}$ is the leading symbol of this operator. Note that its horizontal and vertical derivatives vanish. The equality of the leading symbols of A and $\tilde{A}$ now follows from Proposition 28.

Let a^U denote the local symbol of A in a geodesic coordinate chart U centered at a given point x. We use normal coordinates centered at x. Assume a classical, $h^k a = a_0 + h a_1 + \mathbb{O}(h^2)$. Then a^U is classical, and $h^k a^U = a_0 + \mathbb{O}(h)$. Moreover, it follows from Lemma 26 that $h^k a^U = a_0 + h a_1 + \mathbb{O}(h^2)$ at x. The subprincipal symbol equals, by definition, $h^{1-k}(a_1 + 2^{-1} i \sum_j \partial^2 a_0 / \partial x_j \partial \xi_j)$. The horizontal derivative in the j-th coordinate direction equals, at x, the partial derivative with respect to x_j. The formula for the subprincipal symbol follows. □

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