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MICROLOCAL MOMENTS AND REGULARITY OF SOLUTIONS OF SCHRÖDINGER'S EQUATION

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Abstract. There is a connection between the smoothness of solutions of Schrödinger's equation and the moments of the initial data. This relationship is microlocal in character, and extends on asymptotically flat Riemannian manifolds to a connection between the global scattering behavior of the geodesic flow, the moments of initial data properly microlocalized along bicharacteristics, and the microlocal regularity of the solution. A proof of these results involves an interesting class of symbols of pseudodifferential operators. This article gives an outline of the above results and the microlocal analysis of these symbols. It also contains a study of the evolution operator for the Schrödinger equation on weighted Sobolev spaces, and presents a series of results for the non-selfadjoint case. This article is an extension of seminar talks on the linear Schrödinger equation given at the Ecole Polytechnique on 9 April 1996 (séminaire 'équations aux dérivées partielles') and at the Universität Bonn on 2 May 1996 ('Oberseminar zur Analysis').

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§1. Introduction

This paper considers solutions of the Schrödinger equation in the form

$$
\begin{aligned}
i\partial_t \psi &= -\tfrac{1}{2} \sum_{j,\ell=1}^{n} \partial_{x_j} a^{j\ell}(x) \partial_{x_\ell} \psi \ , \quad x \in \mathbb{R}^n \ , \ t \in \mathbb{R} \ , \\
\psi(x,0) &= \psi_0(x) \ .
\end{aligned} \tag{1}
$$

Our focus is on the moments and the regularity of the initial data $\psi_0(x)$ for equation (1), and their relationship to the moments and the regularity of the solution. The basic fact is that there is a relation between the moment properties of the initial data and the smoothness of the solution for nonzero times t, which depends on the global behavior of the orbits of the classical limit of (1). This latter is the hamiltonian system for $(x,\xi) \in T^*(\mathbb{R}^n)$

$$
\begin{aligned}
\frac{dx}{ds} &= \partial_\xi a(x,\xi) \ , \\
\frac{d\xi}{ds} &= -\ \partial_x a(x,\xi) \ ,
\end{aligned} \tag{2}
$$

with hamiltonian given by the principal symbol of (1);

$$
a(x,\xi) = \tfrac{1}{2} \sum_{j,\ell=1}^{n} a^{j\ell}(x) \xi_j \xi_\ell \ , \tag{3}
$$

whose solution gives the bicharacteristic flow $\varphi(s;x,\xi)$ on the cotangent space $T^*(\mathbb{R}^n)$.

This relationship is clearly a microlocal phenomenon, and the analysis extends to equations of the more general form

$$
i\partial_t \psi = -\tfrac{1}{2} \sum_{j,\ell=1}^{n} \partial_{x_j} a^{j\ell}(x) \partial_{x_\ell} \psi + m_1(x,D)\psi + v_0(x,D)\psi \ , \tag{4}
$$

which includes potential terms, as well as possible first-order terms which would stem from the presence of a magnetic field. The principal results for these equations are described in articles [6] and [4]. In this paper, I extend the analysis in several directions. This includes the study of the mapping properties of the evolution of (1) and (4) on Sobolev and weighted Sobolev spaces, and the extension of certain of the results of the above references to non selfadjoint problems.

To explain the phenomenon, it is best to start with the case of the free Schrödinger equation

$$
i\partial_t \psi = -\tfrac{1}{2} \Delta \psi \ , \quad x \in \mathbb{R}^n . \tag{5}
$$

The following result is well-known, and straightforward to verify.

Theorem 1. *Consider initial data $\psi_0(x) \in L^2(\mathbb{R}^n)$ for equation (5).*
(i) For all $t \in \mathbb{R}$

$$\|\psi(x,t)\|_{L^2} = \|\psi_0(x)\|_{L^2} \ . \tag{6}$$

(ii) If in addition the initial data is localised in the sense that all of its moments are finite,

$$\forall k \ , \quad \int |x^k \psi_0(x)|^2 dx < +\infty \ , \tag{7}$$

then for all $t \neq 0$, the solution $\psi(x,t)$ is C^∞.
(iii) For initial data $\psi_0 \in H^r(\mathbb{R}^n)$, the Sobolev space with norm

$$\|\psi_0(x)\|^2_{H^r} = \int |(1-\Delta)^{r/2}\psi_0(x)|^2 dx \ ,$$

then for all t, $\psi(x,t) \in H^r(\mathbb{R}^n)$, and $\|\psi(x,t)\|_{H^r} = \|\psi_0(x)\|_{H^r}$.
(iv) When $\psi_0(x)$ is in $\mathcal{S}$, the Schwartz class, then for all t, $\psi(x,t)$ is in $\mathcal{S}$.

Statement (i) is fundamental in the interpretation of quantum mechanics, where the measure $|\psi_0(x)|^2dx = dP_0(x)$ describes the initial spatial probability distribution of a quantum particle, $|\psi(x,t)|^2dx = dP_t(x)$ is the spatial distribution that quantum mechanics permits us to deduce at another time t through solution of the Schrödinger equation, and (6) is the fact that the Schrödinger equation (5) preserves probability. Based on this interpretation, it is natural to impose the moment condition (7) on the initial distribution, and the result of Theorem 1(ii) is that the solution is instantaneously smooth, however not necessarily localised, for any nonzero time t. It is distinctly not true that the finiteness of the initial moments alone will guarantee that they are finite at later time; this will be discussed further below. On the other hand, a finite Sobolev norm of $\psi_0(x)$ corresponds directly to finite moments of the momentum density $|\widehat{\psi_0}(\xi)|^2 d\xi$, and the assertion of Theorem 1(iii) is that these moments are preserved by the Schrödinger evolution.

The goal is to study analogous results for solutions of equation (1), and to describe the connection between the dispersive smoothing of solutions and the global behavior of its bicharacteristics from (3). For this purpose we will assume the following estimates on the coefficients of (1):

$$\frac{1}{C}|\xi| \leq |\partial_\xi a(x,\xi)| \leq C|\xi| \ , \tag{8}$$

which is the statement of ellipticity, and

$$|\partial_x^\alpha (a^{j\ell}(x) - \delta^{j\ell})| \leq \frac{C_\alpha}{\langle x\rangle^{\tau(\alpha)}} \ , \quad \tau(\alpha) > |\alpha| + 1 \ , \tag{9}$$

which is the condition that the metric on $\mathbb{R}^n$ given by $(a^{j\ell})^{-1}$ is asymptotically flat.

Definition 2. The point $(x_0, \xi^0) \in T^*(\mathbb{R}^n)$ is not trapped *forwards* (respectively *backwards*) by the bicharacteristic flow if

$$|\pi_x \varphi(s; x_0, \xi^0)| \to \infty \ , \ \text{as } s \to +\infty \ \ (\text{respectively, } s \to -\infty) \ . \tag{10}$$

The set of $(x, \xi) \in T^*(\mathbb{R}^n)$ which is not trapped forwards will be called $\mathcal{E}_+$, and the set which is not trapped backwards will be $\mathcal{E}_-$. The involution $\xi \mapsto -\xi$ of $T^*(\mathbb{R}^n)$ exchanges $\mathcal{E}_+$ and $\mathcal{E}_-$.

The basic result of paper [6] considers the classical wave front set $WF(\psi(x,t))$ of solutions of equation (1).

Theorem 3. *Consider solutions of equation (1) , where the coefficients satisfy the estimates (8) and (9). Suppose that the point (x_0, ξ^0) is not trapped backwards by the bicharacteristic flow $\varphi(s; x, \xi)$. For initial data $\psi_0(x) \in L^2(\mathbb{R}^n)$ which has all of its moments finite (7), then for all $t > 0$, $(x_0, \xi^0) \notin WF(\psi(x,t))$.*

Clearly, the analogous result holds for $t < 0$, whenever (x_0, ξ^0) is not trapped forwards by the bicharacteristic flow.

In addition, it is usual to consider equation (5) with potential or electromagnetic vector potential terms, and for this purpose a similar theorem holds for the more general equation (4), where $m_1(x, \xi)$ and $v_0(x, \xi)$ are symbols of pseudodifferential operators whose properties will be described below. The original work on the microlocal smoothness of Schrödinger's equation (1), (4) is by L. Boutet de Monvel [2] and R. Lascar [12]. The principal work on the microlocal regularity of solutions for $t \neq 0$ depending upon global non trapping conditions on bicharacteristics appears in [6]. The present paper describes these results and gives an outline of the methods used in the proof. In addition, this paper will expand upon [6] in several ways. (i) The first involves global estimates of the moments of solutions in terms of the moments as well as Sobolev norms of the initial data. One corollary of Theorem 1 is that, unlike the solutions of diffusion equations, the moments of solutions of Schrödinger's equation are not able to be bounded in terms of moments alone of the initial data $\psi_0(x)$, and some information about the derivatives of $\psi_0(x)$ is also needed. Necessary and sufficient bounds in terms of weighted Sobolev norms are given in Theorem 14 of Section 3, along with estimates on the growth in time of these moments. (ii) The analysis of [6] extends to the Laplace-Beltrami operator $\sqrt{\det(a)} \sum_{j,\ell} \partial_{x_j} \sqrt{\det(a)^{-1}} a^{j\ell}(x) \partial_{x_\ell}$, but it excludes non selfadjoint operators in equation (1). Using the idea of a gauge transformation which appears in the paper [11], part of the analysis will be performed for suitably decaying non selfadjoint terms in equation (4). This gauge transformation is based upon a microlocal quadrature and the resulting pseudodifferential operators have novel symbol properties, and can be analysed using the techniques of [5, Section 4] and [4]. (iii) Finally, we analyse the mapping properties on Sobolev spaces and weighted Sobolev spaces of the pseudodifferential operators that are analysed in (ii).

The paper [4] and the present paper are completions of the text of seminar talks in Toronto in 1995 and at the Ecole Polytechnique and the Universität Bonn in 1996. While the introductions to both of these are expository, I have tried to minimise the overlap between them, and there are new results in each. A preliminary version (in french) of this article appears in the collection Séminaire Equations aux Dérivées Partielles, 1995 - 1996 (Ecole Polytechnique) [5]. Concerning section 4 of the present article, I would like to thank L. Vega for his friendly and illuminating discussion of his preprint [11].

§2. Microlocal moments and regularity

Rewrite the equation (1) symbolically as

$$i\partial_t \psi = A\psi \ , \tag{11}$$

with $A = -\frac{1}{2}\sum_{j,\ell}\partial_{x_j} a_{j\ell}\partial_{x_\ell}$ selfadjoint on a suitable domain in $L^2(\mathbb{R}^n)$. There is an identity which is satisfied by solutions of (11), for virtually any operator B;

$$\partial_t \mathrm{re}\,\langle\psi, B\psi\rangle + \mathrm{re}\,\langle\psi, \tfrac{1}{i}[A,B]\psi\rangle = \mathrm{re}\,\langle\psi, (\partial_t B)\psi\rangle \ . \tag{12}$$

In the specific cases in which B commutes with A and is time-independent, we conclude that $\partial_t \mathrm{re}\,\langle\psi, B\psi\rangle = 0$. In particular, for $B = I$, then $\partial_t\|\psi(x,t)\|^2_{L^2} = 0$, which exhibits conservation of probability and is the analog of Theorem 1(i) for equation (1). The second basic estimate comes from the choice $B = A$ itself, whereupon $\partial_t\frac{1}{2}\int\sum_{j,\ell} a^{j\ell}(x)\overline{\partial_{x_j}\psi}\partial_{x_\ell}\psi \; dx = 0$, which is the principle of conservation of energy.

Changing the setting somewhat, consider identity (12) using $B = b(x,D)$ a pseudodifferential operator, whose symbol $b(x,\xi)$ is of order m and lies in an appropriate class. The order of the terms appearing in the identity is well defined, and we see that $b(x,D)$ is of order m, while $\frac{1}{i}[A, b(x,D)] = -\{a,b\}(x,D) + e$, where the Poisson bracket is of order $m+1$ and the error will be expected to be of order m or less. The identity (12) will give a useful estimate of the solution if

$$\begin{aligned} c(x,\xi) &= -\ \{a,b\}(x,\xi)\ , \\ b(x,\xi) &\geq 0\ , \quad c(x,\xi) \geq 0\ , \end{aligned} \tag{13}$$

using the Gårding inequality and the differential inequality which results from (12). Equation (13) relating $b(x,\xi)$ and $c(x,\xi)$ is known as the cohomological equation of the dynamical system (2). In fact this is the same strategy used by L. Hörmander in one of his proofs of the theorem of propagation of singularities for solutions of hyperbolic equations; this appeared in [9]. However, in the present case the term $\{a,b\}$ is the principal contribution, and not the error term, as in that reference.

The identity (12) and the demands of positivity (13) bring us to a fundamental question. When can one have a pair of symbols $(b(x,\xi), c(x,\xi))$ satisfying (13)? In other words, statement (13) is that $b(x,\xi) \geq 0$, and $b(x,\xi)$ decreases along the orbits of the bicharacteristic flow of the hamiltonian field (2) of $a(x,\xi)$. A minimal response is that for $s < 0$, $\varphi(s; \mathrm{supp}\,(b)) \subseteq \mathrm{supp}\,(b)$, a relationship which has dire consequences for the symbol properties of $b(x,\xi)$ in the forward scattering regions $\mathcal{E}_+$.

In fact, take the point of view that, given an appropriate symbol $c(x,\xi)$, we will construct the symbol $b(x,\xi)$ such that $-\{a,b\} = -X_a(b) = c$, where X_a is the hamiltonian vector field of $a(x,\xi)$ on $T^*(\mathbb{R}^n)$. It is well known that the existence and regularity of the cohomological equation (13) is very closely related to the recurrence properties of the flow $\varphi(s;x,\xi)$. For the simplest example, if $c(x_0,\xi^0) > 0$ for a point (x_0,ξ^0) on a periodic bicharacteristic, then there cannot be a solution $b(x,\xi)$ of (13).

On the other hand, when $\mathrm{supp}\,(c) \subseteq \mathcal{E}_-$ is in a scattering region, the answer is more straightforward. Take $c(x,\xi) \in S^{m+1}$ a classical symbol, which means that $\pi_x \mathrm{supp}\,(c)$ is compact in $\mathbb{R}^n$, and

$$|\partial_x^\alpha \partial_\xi^\beta c(x,\xi)| \le C_{\alpha\beta} \langle \xi \rangle^{m+1-|\beta|} \ , \tag{14}$$

where the traditional notation in this subject is that $\langle \xi \rangle^2 = (|\xi|^2 + 1)$. Suppose that $\mathrm{supp}\,(c) \subseteq \mathcal{E}_-$ and, to avoid difficulties, that $c(x,\xi) = 0$ for $|\xi| \le 1$. A solution of (13) is obtained by quadrature

$$b(x,\xi) = \int_0^{+\infty} c(\varphi(s;x,\xi))ds \ . \tag{15}$$

Here is the rub; the symbol $b(x,\xi)$ does not have $\pi_x \mathrm{supp}\,(b)$ compact, for its support is along all backwards bicharacteristics which emanate from $\mathrm{supp}\,(c)$. Furthermore, this natural construction (15) does not give rise to a particularly well behaved class of symbols.

Proposition 3. *For $c(x,\psi) \ge 0$ (not identically zero), with* $\mathrm{supp}\,(c) \in \mathcal{E}_-$*, the symbol b constructed by quadrature (15) has* $\pi_x \mathrm{supp}\,(b)$ *not compact. The general symbol estimates that $b(x,\xi)$ satisfies are that*

$$|\partial_x^\alpha \partial_\xi^\beta b(x,\xi)| \le C_{\alpha\beta} \langle \xi \rangle^{m-|\beta|} \langle x \rangle^{+|\beta|} \ . \tag{16}$$

Estimate (16) alone does not give rise to a reasonable symbol class, and pseudo-differential operators constructed from them do not in general form a usual calculus. Fortunately there are several additional properties of symbols which are the result of the process of quadrature. Because $a(x,\xi)$ is asymptotically flat, there are four special vector fields with respect to which the symbol $b(x,\xi)$ is better behaved. Define

$$X_1 = \xi \cdot \partial_\xi \ , \quad X_2 = x \cdot \partial_x \ , \quad X_3 = \frac{\langle \xi \rangle}{\langle x \rangle} x \cdot \partial_\xi \ , \quad X_4 = \frac{\langle x \rangle}{\langle \xi \rangle} \xi \cdot \partial_x \ . \tag{17}$$

Proposition 4. *For classical symbols $c(x,\xi) \in S^{m+1}$ with* $\mathrm{supp}\,(c) \subseteq \mathcal{E}_-$*, then the result $b(x,\xi)$ of quadrature (15) satisfies the estimate*

$$|X^\gamma \partial_x^\alpha \partial_\xi^\beta b(x,\xi)| \le C_{\alpha\beta\gamma} \langle \xi \rangle^{m-|\beta|} \langle x \rangle^{+|\beta|} \ , \tag{18}$$

where α,β are n multiindices, and γ is a 4 multiindex.

Definition 5. The symbol class $S^{m,k}(\rho,\delta)$ consists of those $b(x,\xi) \in C^\infty(\mathbb{R}^n)$ which satisfy

$$|\partial_x^\alpha \partial_\xi^\beta b(x,\xi)| \le C_{\alpha\beta} \langle \xi \rangle^{m-|\beta|} \langle x \rangle^{k+\rho|\beta|-\delta|\alpha|} \ . \tag{19}$$

Define the symbol class $S_d^{m,k}(1,0)$ to be the subclass of $S^{m,k}(1,0)$ which in addition satisfy the analogue of estimate (18) with respect to the vector fields X_j, which is

$$|X^\gamma \partial_x^\alpha \partial_\xi^\beta b(x,\xi)| \le C_{\alpha\beta\gamma} \langle \xi \rangle^{m-|\beta|} \langle x \rangle^{k+|\beta|} \ .$$

For $m = 0$ the operator $b(x,D)$ whose symbol satisfies (16) may not even be bounded on $L^2(\mathbb{R}^n)$, however the operators which result from the process of quadrature are somewhat better behaved.

Theorem 6. *Consider* $c(x,\xi) \in S^1$ *a classical symbol, with* supp $(c) \subseteq \mathcal{E}_-$ *and* $c(x,\xi) = 0$ *for* $|\xi| \le 1$. *Then the solution* $b(x,\xi)$ *of (15) satisfies* $b(x,\xi) \in S_d^{0,0}(1,0)$, *and furthermore*

$$\|b(x,D)\psi(x)\|_{L^2} \le C\|\psi(x)\|_{L^2} \ . \tag{20}$$

The proof of this theorem appears in [6] (section 4); it involves the following steps. (i) Without loss of generality, we can assume that the support of $c(x,\xi)$ is small. (ii) Then one can see that the support of $b(x,\xi)$ from (15) will satisfy the geometric condition that for some constant $R > 0$, whenever both $(x,\xi), (y,\xi) \in$ supp (b) and $|x-y| \ge R$ then

$$\tfrac{1}{2}\langle x-y\rangle|\xi| \le |(x-y)\cdot\xi| \ . \tag{21}$$

This reverse Cauchy - Schwartz inequality implies that within the support of $b(x,\xi)$ the position vectors $(x-y)$ tend asymptotically to align with the momentum ξ; this is precisely the situation for orbits of (2) in either of the classical scattering sets $\mathcal{E}_\pm$. The operator $b(x,D)$ now permits an almost orthogonal decomposition in the backwards scattering region. Clearly the same analysis applies to symbols $c(x,\xi) \in S^{m+1}$ with supp $(c) \subseteq \mathcal{E}_+$ the forward scattering region, with the quadrature formula along the forward bicharacteristic

$$b(x,\xi) = -\int_{-\infty}^{0} c(\varphi(s;x,\xi))\, ds \ , \tag{22}$$

although now $b(x,\xi) \le 0$ if $c(x,\xi) \ge 0$. An immediate application of Theorem 6 and the identity (12) is a 'microlocal smoothing' result for the scattering regions $\mathcal{E}_+ \cup \mathcal{E}_-$ for equation (1).

Theorem 7. *Consider any classical symbol* $s(x,\xi) \in S^{1/2}$ *such that* $\operatorname{supp}(s) \subseteq \mathcal{E}_+ \cup \mathcal{E}_-$. *Let* $\psi(x,t)$ *be a solution of equation (1). For any* $T > 0$, $\psi(x,t)$ *satisfies the estimate*

$$\int_0^T \|s(x,D)\psi(x,t)\|_{L^2}^2 \, dt \le C(T)\|\psi_0(x)\|_{L^2}^2 \ . \tag{23}$$

Proof. We have already observed that the evolution under equation (1) preserves the L^2-norm of solutions. Using smooth cutoff functions it is possible to assume that $s(x,\xi)$ is supported away from $\xi = 0$, and in one of $\mathcal{E}_-$, $\mathcal{E}_+$. Set $c(x,\xi) = s(x,\xi)^2$ and solve (15) or possibly (22) for $b(x,\xi) \in S_d^{0,0}(1,0)$. Use the pair of symbols $(b(x,\xi), c(x,\xi))$ for pseudodifferential operators in the identity (12), and integrate it over the time interval $t \in [0,T]$, giving

$$\begin{aligned} \operatorname{re}\langle\psi(T), b(x,D)\psi(T)\rangle \ + \int_0^T \operatorname{re}\langle\psi(t), -\{a,b\}(x,D)\psi(t)\rangle \, dt \\ = \operatorname{re}\langle\psi_0, b(x,D)\psi_0\rangle \ - \int_0^T \operatorname{re}\langle\psi(t), e\psi(t)\rangle \, dt \ . \end{aligned} \tag{24}$$

The following terms of (24) are bounded in terms of the initial data:

$$\begin{aligned} |\operatorname{re}\langle\psi(T), b(x,D)\psi(T)\rangle| &\le C\|\psi(T)\|_{L^2}^2 = C\|\psi_0\|_{L^2}^2 \\ |\operatorname{re}\langle\psi_0, b(x,D)\psi_0\rangle| &\le C\|\psi_0\|_{L^2}^2 \ . \end{aligned} \tag{25}$$

With some more work ([6], Theorem 4.5) we can show that

$$|\operatorname{re}\langle\psi(t), e\psi(t)\rangle| \le C\|\psi_0\|_{L^2}^2 \ , \tag{26}$$

therefore from (24) we have the estimate of the remaining term

$$\int_0^T \operatorname{re}\langle\psi(t), c(x,D)\psi(t)\rangle \, dt \le C(T)\|\psi_0\|_{L^2}^2 \ , \tag{27}$$

and with an application of the Gårding inequality for the classical symbol $c(x,\xi)$, the result (23) follows. □

For $(x_0,\xi^0) \in \mathcal{E}_-$ and $s(x,\xi)$ constructed with its support in a sufficiently small neighborhood of (x_0,ξ^0), statement (23) is the initial step in an induction argument that gives the result of Theorem 2 of the dispersive smoothing of solutions of equation (1). To obtain the rest of the C^∞ result we have to work harder, with more suitable symbol classes. These will be the classes $S^{m,k}(\rho,\delta)$ of Definition 5, where we take $0 \le \rho < \delta \le 1$, with symbols supported in suitable neighborhoods of the backwards bicharacteristics through (x_0,ξ^0).

Theorem 8. *For $0 \le \rho < \delta \le 1$ the classes $S^{m,k}(\rho,\delta)$ form the basis of a traditional calculus of pseudodifferential operators.*

Symbols with mixed spatial and Fourier transform properties have been studied in the past, in particular in the classical papers of R. Beals & C. Fefferman [1] and in L. Hörmander's paper on the Weyl calculus [10]. The classes $S^{m,k}(\rho,\delta)$ do not satisfy the criteria of [1], however they are a subcase of the Hörmander - Weyl theory. A straightforward independent treatment is presented in [6] and [4].

Given a pair of symbols $(b(x,\xi), c(x,\xi))$ such that $c(x,\xi) = -\{a,b\}(x,\xi)$, and writing $\frac{1}{i}[A, b(x,D)] = -\{a,b\}(x,D) + e$, the time integral of the identity (12) gives that

$$\begin{aligned} &\mathrm{re}\,\langle \psi(T), b(x,D)\psi(T)\rangle + \int_0^T \mathrm{re}\,\langle \psi(t), c(x,D)\psi(t)\rangle\, dt \\ &\qquad = \mathrm{re}\,\langle \psi_0, b(x,D)\psi_0\rangle + \int_0^T \mathrm{re}\,\langle \psi(t), (\dot b(x,D) - e)\psi(t)\rangle\, dt\ . \end{aligned} \tag{28}$$

The first concern is whether suitably microlocalised moments of the solution $\psi(t), t > 0$ can be controlled in terms of the analogous moments of the initial data. Consider a symbol pair $(b_0(x,\xi), c_0(x,\xi)) \in S^{0,K}(\rho,\delta) \times S^{1,K-1}(\rho,\delta)$, with $\rho < \delta$, such that $(x_0,\xi^0) \in \mathrm{supp}\,(c_0) \subseteq \mathrm{supp}\,(b_0) = \mathcal{E}_0 \subseteq \mathcal{E}_-$, and such that

$$\begin{aligned} b_0(x,\xi) &\ge 0\ , \\ c_0(x,\xi) &= -\{a,b_0\}(x,\xi) \ge 0\ , \\ -\{a, \langle x\rangle^{-K} b_0\} &\ge 0 \quad \text{for} \quad |x| \ge R\ . \end{aligned} \tag{29}$$

Such symbol pairs can be constructed when additionally $\rho + \delta > 1$. The error terms of the right hand side of (28) satisfy $\partial_t b = 0$ and $e = e_{(1)}(x,D) + R_{(1)}$, where $e_{(1)}$ is a symbol in the class $S^{0,K-2(\delta-\rho)}(\rho,\delta)$ and $R_{(1)}$ is bounded on $L^2(\mathbb{R}^n)$. Therefore the K-th moments of the solution $\psi(x,T)$, microlocalised within $\mathcal{E}_0$, are bounded in terms of microlocalised K-th moments of the initial data, and $K - 2(\delta-\rho)$ moments of the solution, in a slightly larger neighborhood $\mathcal{E}_1$. Since $K - 2(\delta - \rho) < K$, an iteration on an increasing sequence of neighborhoods of the backwards bicharacteristic $\{(x,\xi) = \varphi(s; x_0, \xi^0)\ :\ s < 0\} \subseteq \mathcal{E}_0 \subseteq \mathcal{E}_1 \cdots \mathcal{E}_m \subseteq \mathcal{E}^{(0)} = \mathrm{supp}\,(s_0)$ serves to prove that the K-th moments of the incoming components of the solution $\psi(x,t)$ are bounded in terms of K-th moments of the initial data $\psi_0(x)$. This is the statement of the following theorem.

Theorem 9. *Suppose that $(x_0,\xi^0) \in \mathcal{E}_-$, then there is a symbol $s_0(x,\xi) \in S^{0,K}(\rho,\delta)$, with $0 \le \rho < \delta \le 1$, $1 \le \rho + \delta$ such that $s(x_0,\xi^0) = 1$ and $b_0(x,\xi) = s_0^2(x,\xi)$ satisfies*

$$\begin{aligned} &-\{a, b_0\}(x,\xi) \ge 0\ , \\ &-\{a, b_0\langle x\rangle^{-K}\}(x,\xi) \ge 0 \quad \textit{for} \quad |x| > R\ . \end{aligned} \tag{30}$$

For initial data $\psi_0(x) \in L^2(\mathbb{R}^n)$ such that its microlocal K-th moments within $\mathrm{supp}\,(s_0) = \mathcal{E}^{(0)}$ *are finite,*

$$\langle \psi_0, s_0^* s_0(x,D)\psi_0\rangle < +\infty\ , \tag{31}$$

then there is a neighborhood $\mathcal{E}^{(1)} \subseteq \mathcal{E}^{(0)}$ containing the backwards bicharacteristic passing through (x_0, ξ^0) such that for all $T > 0$,

$$\sup_{0 \le t \le T} \operatorname{re} \langle \psi(t), b(x, D)\psi(t) \rangle < +\infty \ , \tag{32}$$

for all $b(x,\xi) \in S^{0,K}(\rho,\delta)$ with $\operatorname{supp}(b) \subseteq \mathcal{E}^{(1)}$.

That is to say, for $t > 0$ the microlocal K-th moments of the solution $\psi(x,t)$ are bounded on slightly smaller neighborhoods of the backwards bicharacteristic through the point (x_0, ξ^0). In fact, this statement of [6] is new even for the free Schrödinger equation (5).

The second task is to use again the identity (12) to recursively exchange moment information of the solution within $\mathcal{E}_-$ for microlocalised estimates of derivatives. For this purpose we consider symbol pairs $(b(x,\xi), c(x,\xi)) \in S^{m,k}(\rho,\delta) \times S^{m+1,k-1}(\rho,\delta)$, with $\operatorname{supp}(c) \subseteq \operatorname{supp}(b) \subseteq \mathcal{E}^{(1)} \subseteq \mathcal{E}_-$ such that they satisfy relationships (13). Using the operators $t^p b(x,D)$, $t^p c(x,D)$ in the identity (12), the result is that

$$\begin{aligned} &\operatorname{re} \langle \psi(T), T^p b(x,D)\psi(T) \rangle + \int_0^T \operatorname{re} \langle \psi(t), t^p c(x,D)\psi(t) \rangle \, dt \\ &\quad = \operatorname{re} \langle \psi_0, t^p|_{t=0} b(x,D)\psi_0 \rangle + \int_0^T \operatorname{re} \langle \psi(t), (p t^{p-1} b(x,D) - t^p e)\psi(t) \rangle \, dt \ . \end{aligned} \tag{33}$$

When $p > 0$ the first term of the RHS vanishes, and the identity does not depend explicitly upon the initial data $\psi_0(x)$. For the n-th induction step, take $m = n$, $p = n$ and $k = K - n$, whereupon the LHS of (33) is bounded in terms of time integrals of quantities involving lower numbers of derivatives and lower powers of t, but higher moments. The result is paraphrased in a theorem which states the gain of microlocal derivatives of the solution in terms of the microlocalised moment properties of the initial data.

Theorem 10. *Suppose that $(x_0, \xi^0) \in T^*(\mathbb{R}^n)$ is not trapped backwards by the bicharacteristic flow of the principal symbol $a(x,\xi)$. In appropriate slightly smaller neighborhoods $\mathcal{E}^{(2)} \subseteq \mathcal{E}^{(1)} \subseteq \mathcal{E}_-$ of the backwards bicharacteristic through (x_0, ξ^0), consider symbol pairs $(b_K(x,\xi), c_K(x,\xi)) \in S^{K,0}(\rho,\delta) \times S^{K+1,-\nu}(\rho,\delta)$ (with $\nu > 1$), such that relationships (13) are satisfied. Consider initial data $\psi_0(x)$ such that*

$$\langle \psi_0, s_0^* s_0(x,D)\psi_0 \rangle < +\infty \ , \tag{34}$$

then for all $T > 0$ and $K' > K$ ($K' = K$ if K is an integer),

$$\begin{aligned} &\sup_{0 \le t \le T} t^{K'} \operatorname{re} \langle \psi(t), b_K(x,D)\psi(t) \rangle < +\infty \ , \\ &\int_0^T t^{K'} \operatorname{re} \langle \psi(t), c_K(x,D)\psi(t) \rangle \, dt < +\infty \ . \end{aligned} \tag{35}$$

This statement makes precise the additional microlocal smoothness that one may expect near nontrapped points (x_0, ξ^0), in terms of the microlocal moment properties of the initial data within the neighborhoods $\mathcal{E}^{(1)} \subseteq \mathcal{E}^{(0)}$ of the backwards bicharacteristic through (x_0, ξ^0). This result, which appears in [6] is also new even for the free Schrödinger equation (5). In cases where $(x_0, \xi^0) \in \mathcal{E}_-$ is also not trapped by the forwards bicharacteristic flow, a similar induction argument is available which gives bounds on the asymptotic growth at spatial infinity of the derivatives of the outgoing components of the solution. In this case it is necessary to consider symbol pairs $(b_n(x,\xi), c_n(x,\xi)) \in S_d^{m,k}(1,0) \times S_d^{m+1,k-1}(1,0)$, with the induction using $n = m \le K$, $p = n$ and with $k < -n$ negatively weighted in $\langle x \rangle$. Indeed, the solution is as smooth as the number of incoming moments allows, however the size of the derivatives of the solution grows in $\langle x \rangle$.

Under the involution $\xi \mapsto -\xi$, the sets $\mathcal{E}_+$ and $\mathcal{E}_-$ are exchanged, and under analogous conditions, the same results hold for $t < 0$. A simple modification of the proof works for the equation (4), under the conditions on the two symbols $m_1(x,\xi), v_0(x,\xi)$ that $m_1(x,\xi)$ is real, and that for some $p < 1$,

$$\begin{aligned} &|\partial_x^\alpha \partial_\xi^\beta m_1(x,\xi)| \le C_{\alpha\beta} \langle \xi \rangle^{1-|\beta|} \langle x \rangle^{p-|\alpha|} \ , \\ &|\partial_x^\alpha \partial_\xi^\beta v_0(x,\xi)| \le C_{\alpha\beta} \langle \xi \rangle^{1-|\beta|} \langle x \rangle^{p-1-|\alpha|} \ . \end{aligned} \tag{36}$$

A real potential $v(x)$ which satisfies $|\partial_x^\alpha v(x)| \le C_\alpha \langle x \rangle^{p-|\alpha|}$ is permitted by hypothesis (36), as it satisfies the estimates for $m_1(x,\xi)$. This is discussed in references [6], [3] and [4]. Further information on the growth rate of the potential terms and the smoothness of the kernel for Schrödinger's equation is given in the discussion in [3].

There have been some recent results addressing the expected lack of smoothness of solutions to (1) corresponding to trapped classical orbits. In particular S. Doi [7] has shown that if (x_0, ξ^0) is recurrent under the flow $\varphi(s)$, then estimate (23) cannot hold for all $s(x,\xi) \in S^{1/2}$ supported in a neighborhood of (x_0, ξ^0). He has further proved that (23) holds along nontrapped classical orbits for both asymptotically euclidian and asymptotically hyperbolic noncompact manifolds. Perhaps the best heuristic argument for the existence of singularities of solutions along recurrent orbits is the explicit solution for the circle. Consider equation (5) for $x \in [0, 2\pi)$, with periodic boundary conditions, where the Schrödinger kernel is

$$S_p(x-y,t) = \frac{1}{2\pi} \sum_k e^{ik(x-y)} e^{-ik^2 t/2} \ .$$

At rational times $t = P/Q$, use the euclidian algorithm to decompose each momentum $k = 2aQ + b$, with $a \in \mathbb{Z}$ and $0 \le b < Q$. The Schrödinger kernel is therefore

$$\begin{aligned} S_p(x-y, P/Q) &= \frac{1}{2\pi} \sum_{a \in \mathbb{Z}} \sum_{0 \le b < Q} e^{2iaQ(x-y)} e^{i(b(x-y) - b^2 P/2Q)} \\ &= \frac{1}{2\pi} \sum_{\substack{0 \le j < Q \\ 0 \le b < 2Q}} e^{i(b(x-y) - b^2 P/2Q)} \delta(x - y - \frac{j}{Q}) \ , \end{aligned}$$

which is singular at Q many points equally spaced about the circle. Even worse, at irrational times t the Schrödinger kernel S_p is not even a measure (personal communication of C. Bardos, P. Gérard and J. Rauch).

§3. Estimates in Sobolev spaces

In this section we will derive the basic mapping properties of the evolution of the Schrödinger equations (1) and (4), on the standard Sobolev spaces and weighted Sobolev spaces. The estimates are global, in the sense that the inspection of solutions and their derivatives does not employ cutoff functions nor microlocal techniques. Furthermore, the estimates are basic; even so they do not appear in the present literature, so far as I know, for the variable coefficient equations considered in [3], [4], [6] and this paper. The hypotheses that we impose on the coefficients of equation (1) are that

$$-\tfrac{1}{2}\sum_{j,\ell=1}^{m} \partial_{x_j} a^{j\ell}(x)\partial_{x_\ell} = a(x,D) + a_1(x,D)\ , \tag{37}$$

where the pseudodifferential operators have symbols $a(x,\xi)$ the principal symbol given in (3), and $a_1(x,\xi) = -\sum_{j,\ell} i\partial_{x_j} a^{j\ell}(x)\xi_\ell$. In terms of symbol classes, we ask that $a(x,\xi) \in S^{2,0}(0,1)$, so that $a_1(x,\xi) \in S^{1,-1}(0,1)$, and that the ellipticity condition holds,

$$\frac{1}{C}|\xi|^2 \le a(x,\xi) \le C|\xi|^2\ . \tag{38}$$

This is weaker than (9) in terms of decay rates, although it still requires the matrix $(a^{j\ell})^{-1}$ to be asymptotically flat. The requirements for the lower order coefficients of equation (4) are that $m_1(x,\xi) \in S^{1,0}(0,1)$ and is real, while $v_0(x,\xi) \in S^{0,0}(0,1)$. It is conceivable that these requirements can be weakened to those of (36), but we will not pursue that here.

Theorem 11. *Solutions of equation (1) conserve probability and conserve energy, that is,*

$$\begin{gathered}\|\psi(x,t)\|_{L^2} = \|\psi_0\|_{L^2} \quad \textit{and} \\ \sum_{j,\ell}\int a^{j\ell}(x)\overline{\partial_{x_j}\psi(x,t)}dx = \langle\psi(t), A\psi(t)\rangle = \langle\psi_0, A\psi_0\rangle\ .\end{gathered} \tag{39}$$

Suppose that $m_1(x,D) + v_0(x,D)$ is formally selfadjoint on $L^2(\mathbb{R}^n)$. Then solutions of equation (4) also conserve probability and energy.

Proof. These facts have already been mentioned above, and the basic idea of the proof is that in the identity (12), the operators $B = I$ and $B = A$ commute with A. Of course, solutions are not necessarily smooth, so the complete proof involves approximations of $L^2(\mathbb{R}^n)$ by smooth solutions and a limit argument. The *energy* for equation (4) is the inner product $\langle\psi(t), (A + m_1(x,D) + v_0(x,D))\psi(t)\rangle$. □

The analogy of Theorem 1(iii) for solution of equations (1) and (4) is the result that evolution preserves the classical Sobolev spaces $H^r(\mathbb{R}^n)$.

Theorem 12. *Solutions of equation (1) preserve the Sobolev estimates on the spaces* $H^r(\mathbb{R}^n)$*,*

$$\|\psi(x,t)\|_{H^r} \le C(r)\|\psi_0(x)\|_{H^r} \ . \tag{40}$$

When $m_1(x,\xi) \in S^{1,0}(0,1)$ *is real and* $v_0(x,\xi) \in S^{0,0}(0,1)$ *then Sobolev estimates hold for solutions of equation (4);*

$$\|\psi(x,t)\|_{H^r} \le e^{C(r)t}\|\psi_0(x)\|_{H^r} \ . \tag{41}$$

Just as moment requirements such as (7) give information about the localisation of the position density $|\psi(x,t)|^2 dx = dP_t(x)$, Sobolev estimates give moment information about the momentum density $|\widehat{\psi}(\xi,t)|^2 d\xi = d\widehat{P}_t(\xi)$. Theorem 12 states that the $2r$-moments of $d\widehat{P}_t(\xi)$ are bounded in terms of $2r$-moments of the initial momentum density $\widehat{dP_0}(\xi)$, whereas the parallel statements for position density are not true. It is natural then to ask for sufficient information so that spatial moments of the solution are controlled; this is the result of the next theorem.

Definition 13. The weighted Sobolev space $W^r(\mathbb{R}^n)$ is the Hilbert space that is the closure of $\mathcal{S}$ with respect to the norm

$$|\psi(x)|^2_{W^r} = \sum_{|\alpha|+|\beta|=r} \int |x^\beta \partial_x^\alpha \psi(x)|^2 dx \ . \tag{42}$$

Theorem 14. *Solutions of equation (1) preserve the weighted Sobolev spaces* $W^r(\mathbb{R}^n)$*. Indeed, they satisfy the estimate*

$$|\psi(x,t)|_{W^r} \le e^{C(r)t}|\psi_0(x)|_{W^r} \ . \tag{43}$$

Solutions of equation (4) will also satisfy (43) when, as before, $m_1(x,\xi) \in S^{1,0}(0,1)$ *is real and* $v_0(x,\xi) \in S^{0,0}(0,1)$*.*

Note in particular that the variance, $\int |x|^2|\psi(x,t)|^2 dx$, of a solution is finite for every $t \in \mathbb{R}$ if the initial data has both finite initial variance and finite initial energy, but not necessarily otherwise. In fact, the solution operators for (1) and (4) also preserve the Hilbert spaces based on the norms

$$|\psi(x)|^2_{(r,s)} = \sum_{0\le|\beta|\le s} |\partial_x^\beta \psi(x)|^2_{W^r} \ .$$

We can also see that the character of the norm (42) is necessary by the following examples of gaussian wave packets. Consider initial data for (5) of the form

$$\psi_0(x) = \exp(-\tfrac{1}{2}(x,ax) + i(k,x)) \ , \tag{44}$$

with $a = a^T$ real and positive definite. Then $dP_0(x) = \exp(-(x,ax))dx$ and $\|\psi_0(x)\|^2_{L^2} = \sqrt{\pi^n/\det(a)}$ (we have not bothered to normalise ψ_0, so that dP_0 is not a probability measure). Moments of $dP_0(x)$ are

$$\int x^m |\psi_0(x)|^2 dx = \int x^m \exp(-(x,ax))dx \ , \tag{45}$$

which are independent of k. Furthermore, weighted Sobolev norms of $\psi_0(x)$ can be expressed:

$$\|\langle x\rangle^p \partial_x^q \psi_0(x)\|^2_{L^2} = \int \langle x\rangle^{2p} P_q(x,k)\exp(-(x,ax))dx \tag{46}$$

with $P_q(x,k)$ a monic polynomial in k of maximal degree $2|q|$. The solution of (5) with data (44) is the gaussian wave packet $\psi(x,t) = \int S^0(x-y,t)\psi_0(y)dy$, for $S^0(x,t)$ the free Schrödinger kernel, and this solution is explicitly

$$\psi(x,t) = \frac{1}{\sqrt{(2\pi i t)^n \det(1+t^2a^2)}} \exp\big(-\tfrac{1}{2}(x-kt, a(1+t^2a^2)^{-1}(x-kt))\big)\exp(i\Phi) \tag{47}$$

where the phase is $\Phi(x,t) = \frac{1}{2t}\big((x,x) - (x-kt,(1+t^2a^2)^{-1}(x-kt))\big)$. The position density is therefore

$$dP_t(x) = \frac{1}{(2\pi t)^n \det(1+t^2a^2)} \exp\big(-(x-kt, a(1+t^2a^2)^{-1}(x-kt))\big)\ dx \ ,$$

which has $2|r|$th moments

$$\int |x^r|^2 dP_t(x) = \frac{1}{(2\pi t)^n \det(1+t^2a^2)} \int |(x+kt)^r|^2 \exp\big(-(x,-a(1+t^2a^2)x)\big)dx \ , \tag{48}$$

and these grow in $|(kt)^r|^2$. The conclusion is that (48) will diverge in k faster than (46) unless explicitly $|q| \ge |r|$, hence moments of the solution $\|\langle x\rangle^r \psi(x,t)\|^2_{L^2}$ will not be bounded in any Sobolev norm of the initial data which does not refer to at least $2|r|$ many moments and $2|r|$ many derivatives.

Proof. (of Theorem 12) Ellipticity of A implies that the norms constructed from the operator A,

$$\begin{aligned} &\langle A^{r/2}\psi, A^{r/2}\psi\rangle + \|\psi\|^2_{L^2} \quad (r \text{ even}) \ , \\ &\langle A^{(r+1)/2}\psi, A^{(r-1)/2}\psi\rangle + \|\psi\|^2_{L^2} \quad (r \text{ odd}) \ , \end{aligned} \tag{49}$$

are comparable to the Sobolev norm of $H^r(\mathbb{R}^n)$. For equation (1), the standard estimate is to take $b(x,D) = A^r$ in identity (13), and this of course commutes with A, giving that $\partial_t\langle\psi(t), A^r\psi(t)\rangle = 0$. Of course, the typical element $\psi \in H^r(\mathbb{R}^n)$ is not smooth, but the usual argument of approximation by smooth functions goes through in this setting, and proves that the quantities in (49) are preserved by the evolution of (1). When lower order terms are included, the same proof goes through, with modifications for the effects of the perturbations.

Lemma 15. *For $m_1(x,\xi) \in S^{1,0}(0,1)$ a real symbol and $v_0(x,\xi) \in S^{0,0}(0,1)$,*

$$
\begin{aligned}
&[A^p, m_1(x,D)] = \tfrac{1}{i}\{a^p, m_1\}(x,D) + e_{(1)} \\
&\big(A^p m_1(x,D) - m_1^*(x,D)A^p\big) = \tfrac{1}{i}\{a^p, m_1\}(x,D) + e_{(2)} \qquad (50)\\
&[A^p, v_0(x,D)] = \tfrac{1}{i}\{a^p, v_0\}(x,D) + e_{(3)}
\end{aligned}
$$

with $\{a^p, m_1\}(x,\xi) \in S^{2p,-1}(0,1)$, $\{a^p, v_0\}(x,\xi) \in S^{2p-1,-1}(0,1)$, and with $e_{(1)}$, $e_{(2)}$ bounded from $L^2(\mathbb{R}^n)$ to $H^{2p-1}(\mathbb{R}^n)$, $e_{(3)}$ bounded from $L^2(\mathbb{R}^n)$ to $H^{2p-2}(\mathbb{R}^n)$.

Proof. The operators $A = a(x,D) + a_1(x,D)$, $m_1(x,D)$ and $v_0(x,D)$ are formed from symbol classes $S^{m,k}(0,1)$, which have a well behaved symbol calculus (see [4] and [5, section 5]). This makes the proof straightforward. □

To finish Theorem 12, suppose that $m_1(x,D)$ and $v_0(x,D)$ are as required. Then for r even, the analog of the identity (13) with $b = A^r$ states

$$
\begin{aligned}
&\partial_t \mathrm{re}\,\langle\psi, A^r\psi\rangle + \mathrm{re}\,\langle\psi, \tfrac{1}{i}[A, A^r]\psi\rangle + \mathrm{re}\,\langle\psi, \big(\tfrac{1}{i}(A^r m_1(x,D) - m_1^*(x,D)A^r) \qquad (51)\\
&\qquad + \tfrac{1}{i}(A^r v_0(x,D) - v_0^*(x,D)A^r)\big)\psi\rangle = 0\ .
\end{aligned}
$$

Of course, $[A, A^r] = 0$ and we estimate the remainder as

$$
\begin{aligned}
&\mathrm{re}\,\langle\psi, \tfrac{1}{i}(A^r m_1(x,D) - m_1^*(x,D)A^r)\psi\rangle \\
&\quad = -\,\mathrm{re}\,\langle A^{r/2}\psi, \tfrac{1}{i}(A^{r/2} m_1(x,D) - m_1^*(x,D)A^{r/2})\psi\rangle \qquad (52)\\
&\qquad + \mathrm{re}\,\langle A^{r/2}\psi, \tfrac{1}{i}(A^{r/2} m_1(x,D) - m_1(x,D)A^{r/2})\psi\rangle\ .
\end{aligned}
$$

The quantities in (52) are the first two expressions in (50) of Lemma 15, and therefore

$$
\begin{aligned}
&\|(A^{r/2} m_1(x,D) - m_1^*(x,D)A^{r/2})\psi\|_{L^2} \le C(r)\|\psi\|_{H^r}\ , \\
&\|(A^{r/2} m_1(x,D) - m_1(x,D)A^{r/2})\psi\|_{L^2} \le C(r)\|\psi\|_{H^r}\ .
\end{aligned}
$$

A simpler estimate holds for the term involving $v_0(x,D)$. Identity (51) therefore gives a differential inequality for $\langle\psi(t), A^r\psi(t)\rangle$ which implies (41). The case r odd is similar. We remark that if $m_1(x,\xi) = 0$ and $v_0(x,\xi)$ is real then (41) holds with a bound which is constant in t rather than growing exponentially, since $\langle\psi, (A+V)^r\psi\rangle \sim \|\psi\|^2_{H^r}$. □

Proof. (of Theorem 14) We will consider equation (1), as the proof for equation (4) involves only extra error terms in the analysis. Given a solution $\psi(x,t)$, then

$$
i\partial_t(\langle x\rangle^q\psi) = A(\langle x\rangle^q\psi) + [\langle x\rangle^q, A]\psi\ . \qquad (53)
$$

Calculating the commutator term,

$$
\begin{aligned}
[\langle x\rangle^q, A]\psi = &-\tfrac{1}{2}\sum_{j,\ell}(\partial_{x_\ell}\langle x\rangle^q)a^{j\ell}(x)\partial_{x_j}\psi - \sum_{j,\ell}(\partial_{x_\ell}a^{j\ell})(\partial_{x_j}\langle x\rangle^q)\psi \qquad (54)\\
&-\tfrac{1}{2}\sum_{j,\ell}a^{j\ell}(x)(\partial_{x_j}\partial_{x_\ell}\langle x\rangle^q)\psi\ .
\end{aligned}
$$

Since $a(x,\xi) \in S^{2,0}(0,1)$, an inspection of the decay rates of the coefficients in (54) gives the following lemma.

Lemma 16.

$$\|\partial_x^r[\langle x\rangle^q, A]\|_{L^2} \le C(r,q)\big(\|\langle x\rangle^{q-1}\partial_x^{r+1}\psi\|_{L^2} + \|\langle x\rangle^{q-2}\partial_x^r\psi\|_{L^2} + \cdots + \|\langle x\rangle^{q-r}\psi\|_{L^2}\big) \ .$$

This is not sufficient to use in (53) for a differential inequality for $\langle x\rangle^q\partial_x^r\psi$, but it gives the information needed for the induction step for Theorem 14.

Lemma 17. *Suppose that $\psi(x,t)$ satisfies the estimate*

$$\|\langle x\rangle^{q-1}\partial_x^{r+1}\psi(x,t)\|_{L^2} \le \exp(C(q-1,r+1)t)\|\langle x\rangle^{q-1}\psi_0\|_{H^{r+1}} \ , \tag{55}$$

then

$$\|\langle x\rangle^q\partial_x^r\psi(x,t)\|_{L^2} \le \exp(C(q,r)t)\big(\|\langle x\rangle^q\partial_x^r\psi_0(x)\|_{L^2} + C(q-1,r+1)\|\langle x\rangle^{q-1}\psi_0\|_{H^r}\big) \ . \tag{56}$$

The proof, as usual, involves the Gronwall inequality for (53), applied to $A^{r/2}\psi$, and the estimate of Lemma 16 to bound the error terms. The induction to prove Theorem 14 starts with the statement of Theorem 12 for $H^r(\mathbb{R}^n)$, and proceeds with descending r and ascending q to give the desired result. □

§4. Non selfadjoint problems

The results of [6] are almost entirely confined to the case where the operator on the RHS of (4) is selfadjoint (only excepting zero order terms which decay in large $\langle x\rangle$). It is natural to ask the extent to which the selfadjoint property is required for the results of dispersive smoothing. The approach in this section involves a so-called gauge transformation, and it is interesting that these transformations are given by pseudodifferential operators based on the symbol class $S_d^{0,0}(1,0)$. In this section, we will consider the general second order equations with variable coefficients, which for convenience are written in the following form:

$$i\partial_t\psi = \big(a(x,D) + a_1(x,D)\big)\psi + \big(m_1(x,D) + ic_1(x,D)\big)\psi + v_0(x,D)\psi \ . \tag{57}$$

Both first order symbols $m_1(x,\xi)$ and $c_1(x,\xi)$ will be taken to be real, $a(x,D) + a_1(x,D) = A$ is selfadjoint as above, and the new term in the problem is the non selfadjoint first order contribution $ic_1(x,D)$. Equation (57) is not necessarily comparable to itself under time reversal, in contrast to equation (1), and our convention will be to continue to discuss the case $t > 0$, however with the warning that it is no longer true that the same results hold for $t < 0$, simply by invoking the involution $\xi \mapsto -\xi$ of $T^*(\mathbb{R}^n)$. The easiest non selfadjoint result for (57) is if there is a dissipative sign condition imposed on $c_1(x,\xi)$.

Theorem 18. *Suppose $c_1(x,\xi) \in S^{1,p}(0,1)$ is real and satisfies $c_1(x,\xi) \ge 0$. Then for $t > 0$ the conclusions of Theorem 3, Theorem 7 and Theorem 10 hold for solutions of (57).*

Proof. For simplicity, set $m_1(x,\xi) = 0 = v_0(x,\xi)$. The identity (13) is modified to be

$$\begin{aligned}\partial_t\mathrm{re}\,\langle\psi, b(x,D)\psi\rangle + &\mathrm{re}\,\langle\psi, \tfrac{1}{i}[a(x,D)+a_1(x,D), b(x,D)]\psi\rangle \\ &+ \langle\psi, \tfrac{1}{2}(bc_1(x,D) + c_1^*(x,D)b)\psi\rangle = \mathrm{re}\,\langle\psi, \partial_t b\psi\rangle \ .\end{aligned}$$

Instead of being a difficult term, the quantity $\frac{1}{2}(bc_1 + c_1^* b(x,D))$ is positive to principal order due to the hypothesis on the sign of $c_1(x,\xi)$. For $b(x,\xi) \in S_d^{0,0}(1,0)$ which satisfies the geometric condition (21),

$$\frac{1}{2}\langle\psi, \big(b(x,D)c_1(x,D) + c_1^*(x,D)b(x,D)\big)\psi\rangle \geq c\|s(x,D)\psi\|_{L^2}^2 + \langle\psi, e_0\psi\rangle \ , \tag{58}$$

where e_0 is an operator bounded on $L^2(\mathbb{R}^n)$. Use this to control the extra term which will appear in the proof of Theorem 7, and the conclusion (27) will follow. Similar considerations can be used in the induction steps in Theorem 10, whence its conclusion and that of Theorem 3 will also follow. □

More interesting analysis comes into play when the symbol $c_1(x,\xi)$ in equation (57) is not assumed to take a particular sign. We may assume that $c_1(x,\xi) = 0$ for $|\xi| \leq 1$ by modifying the term $v_0(x,\xi)$. Consider the transformation $p(x,D)\psi = \varphi$, and its effect upon the equation (57);

$$\begin{aligned} i\partial_t\varphi &= \big(a(x,D) + a_1(x,D)\big)\varphi + m_1(x,D)\varphi + v_0(x,D)\varphi \\ &\quad + \big([p,a] + ip(x,D)c_1(x,D)\big)\psi + [p,(a_1 + m_1 + v_0)]\psi \ . \end{aligned} \tag{59}$$

The idea in [11] is to choose the transformation $p(x,D)$ so that the highest order term of $[p,a] + ipc_1$ vanishes, leaving only a zero order term which is controllable in L^2, and then our analysis goes through. This strategy dictates that

$$\{a,p\}(x,\xi) + p(x,\xi)c_1(x,\xi) = 0 \ , \tag{60}$$

which is to say that,

$$p(x,\xi) = \exp(b_0(x,\xi)) \ , \text{ and } -\{a,b_0\} = c_1(x,\xi) \ . \tag{61}$$

The equation for $b_0(x,\xi)$ is precisely the cohomological equation of the dynamical system (3), whose recurrence properties affect the solvability of (61). There is clearly little hope of simplifying (57) through such transformations, unless the bicharacteristic flow is not trapped on the support of the symbol $c_1(x,\xi)$. Continue, then, under the assumption that $\mathrm{supp}\,(c_1) \subseteq \mathcal{E}_+ \cup \mathcal{E}_-$. From our previous experience of quadrature, we have the following knowledge of the nature of the symbol $p(x,\xi)$.

Proposition 19. *The symbol $b_0(x,\xi)$ obtained from quadrature from $c_1(x,\xi)$ is in the symbol class $S_d^{0,0}(1,0)$. Furthermore, it follows by the Leibniz rule that the symbol $p(x,\xi) = \exp(b_0(x,\xi))$ is in $S_d^{0,0}(1,0)$ as well.*

This class of operators has been studied in [6] and in [4], and here they arise very naturally again, in a new setting. In order that $p(x,\xi)$ satisfy the geometric condition (21), we will adopt the very restrictive assumption that $\pi_x\mathrm{supp}\,(c_1)$ is compact in $\mathbb{R}^n$. It is very likely that less stringent hypotheses may be taken, however we will not pursue that here. We will now assume the following conditions on the coefficients of equation (57).

$$
\begin{aligned}
&a(x,\xi) \text{ is elliptic and asymptotically flat,}\\
&m_1(x,\xi) \in S^{1,0}(0,1) \text{ and is real,}\\
&v_0(x,\xi) \in S^{0,0}(0,1), \text{ and}\\
&c_1(x,\xi) \in S^{1,0}(0,1), \text{ with } \operatorname{supp}(c_1) \subseteq \mathcal{E}_+ \cup \mathcal{E}_-,\\
&\qquad \pi_x \operatorname{supp}(c_1) \subset\subset \mathbb{R}^n \ , c_1(x,\xi) = 0 \text{ for } |\xi| \le 1 \ .
\end{aligned} \tag{62}
$$

Theorem 4.5 of [6] addresses the question of composition of an $S_d^{m,k}(1,0)$-based operator with the more classical $S^{m_1,k_1}(0,1)$ kind, with the following conclusions in our case.

Proposition 20. *The following list of operators are bounded on $L^2(\mathbb{R}^n)$.*

$$
\begin{aligned}
&p(x,D)a(x,D) - a(x,D)p(x,D) + ip(x,D)c_1(x,D) \ ,\\
&p(x,D)a_1(x,D) - a_1(x,D)p(x,D) \ ,\\
&p(x,D)m_1(x,D) - m_1(x,D)p(x,D) \ ,\\
&p(x,D)v_0(x,D) \ ,\\
&v_0(x,D)p(x,D) \ .
\end{aligned}
$$

Denote for the interim the terms of (59) which explicitly involve ψ by f, that is,

$$
\begin{aligned}
f(x,t) =& \big([p(x,D), a(x,D)] + ip(x,D)c_1(x,D)\\
&\quad + [p(x,D), a_1(x,D) + m_1(x,D) + v_1(x,D)]\big)\psi(x,t) \ ,
\end{aligned}
$$

and assume that $\|\psi(x,t)\|_{L^2}$ is finite. It is then relevant to study the inhomogeneous equation

$$
\begin{aligned}
i\partial_t\varphi &= \big(a(x,D) + a_1(x,D)\big)\varphi + m_1(x,D)\varphi + v_0(x,D)\varphi + f(x,t) \ ,\\
\varphi(x,0) &= \varphi_0(x) \in L^2(\mathbb{R}^n) \ , \quad f(x,t) \in L^2(\mathbb{R}^n) \ .
\end{aligned} \tag{64}
$$

This has a treatment in $L^2(\mathbb{R}^n)$ (or indeed in $H^r(\mathbb{R}^n)$ if $f(x,\xi)$ permits) as the homogeneous case (4), and the analog identity to (13) is that

$$
\begin{aligned}
&\partial_t \operatorname{re}\langle\varphi, b(x,D)\varphi\rangle + \operatorname{re}\langle\varphi, \tfrac{1}{i}[a + a_1, b(x,D)]\varphi\rangle\\
&\qquad + \operatorname{re}\langle\varphi, \tfrac{1}{i}\big((b(x,D)m_1 - m_1^* b(x,D)) + (b(x,D)v_0 - v_0^* b(x,D))\big)\varphi\rangle\\
&\quad = \operatorname{re}\langle\varphi, \partial_t b(x,D)\varphi + (b(x,D) - b^*(x,D))f\rangle \ .
\end{aligned} \tag{65}
$$

Under assumptions (62), or even more lenient, this gives Sobolev estimates of solutions of (64) in terms of $\varphi_0(x)$ and $f(x,t)$. In particular, if we set $b(x,D) = I$, then

$$
\partial_t\|\varphi(x,t)\|_{L^2}^2 \le C_0\big(\|\varphi(x,t)\|_{L^2}^2 + \|\varphi(x,t)\|_{L^2}\|f(x,t)\|_{L^2}\big) \ , \tag{66}
$$

therefore

$$\|\varphi(t)\|_{L^2}^2 \leq e^{C_0 t}\|\varphi_0\|_{L^2}^2 + \int_0^t e^{C_0(t-\tau)}\|f(x,\tau)\|_{L^2}^2 d\tau \ . \tag{67}$$

This is not an estimate of (59), since $f(x,t)$ is a linear function of φ through the relation $p(x,D)\psi = \varphi$. Furthermore, we expect the inverse $p^{-1}(x,D)$ to be $q \sim \exp(-b_0(x,D))$, however since there is no pseudodifferential calculus for $S_d^{0,0}(1,0)$ this relationship between $\exp(-b_0(x,D))$ and $p^{-1}(x,D)$ is not guaranteed. Under the hypothesis that $p(x,D)$ is boundedly invertible on $L^2(\mathbb{R}^n)$, we do have the following result.

Theorem 21. *If the operator $p(x,D)$ is boundedly invertible on $L^2(\mathbb{R}^n)$, then there exists a solution $\varphi(x,t)$ of equation (59) in $L^2(\mathbb{R}^n)$, and it satisfies the estimate*

$$\|\varphi(t)\|_{L^2} \leq e^{C_1 t}\|\varphi_0\|_{L^2} \ , \tag{68}$$

where C_1 depends upon C_0 as well as the operator norms of $p^{-1}(x,D)$, $[p,a] + ipc_1$ and $[p, a_1 + m_1 + v_0]$. In this case, $\psi = p^{-1}(x,D)\varphi$ and satisfies the equation (57).

Proof. In outline, use an iteration for $\varphi_n(t)$ which is the solution of (64) with $f = f(\psi_{n-1})$, where $\psi_{n-1} = p^{-1}\varphi_{n-1}$. Straightforward estimates show that this inhomogeneous equation has solutions in $L^2(\mathbb{R}^n)$, and an equally straightforward construction argument involving estimate (67) over a short time interval shows that the sequence $\varphi_n(x,t)$ converges in $\mathcal{C}([0,T]; L^2(\mathbb{R}^n))$ to a solution of (59). □

The identity (65) can be used again to demonstrate a microlocal smoothing estimate for solutions of equation (59), similar to the estimate (23). Assume as above that the coefficients of (57) satisfy (62).

Theorem 22. *Suppose that $p(x,D)$ is boundedly invertible on $L^2(\mathbb{R}^n)$. Consider $c(x,\xi)$ a classical symbol in $\mathcal{S}^1$ such that* supp $(c) \subseteq \mathcal{E}_+ \cup \mathcal{E}_-$. *Then for all $T > 0$, the solution to equation (59) satisfies the microlocal smoothing estimate*

$$\int_0^T \mathrm{re}\,\langle \varphi(t), c(x,D)\varphi(t)\rangle dt \leq C\|\varphi_0\|_{L^2}^2 \ . \tag{69}$$

In this case, the solution $\psi(x,t) = p^{-1}(x,D)\varphi(x,t)$ satisfies the smoothing estimate

$$\int_0^T \mathrm{re}\,\langle \psi(t), \tilde{c}(x,D)\psi(t)\rangle dt \leq C\|\psi_0\|_{L^2}^2 \ , \tag{70}$$

where $\tilde{c}(x,\xi) = |p(x,\xi)|^2 c(x,\xi)$.

Proof. Using identity (65) and solving (14) for $b(x,\xi) \in S_d^{0,0}(1,0)$ given $c(x,\xi) \in \mathcal{S}^1$ with supp $(c) \subseteq \mathcal{E}_+ \cup \mathcal{E}_-$, we can follow the procedure of the proof of Theorem 7 to conclude (69). To obtain (70), we can use the result from [4] that the composition of

$S_d^{m,k}(1,0)$ with a classical symbol (with $\pi_x \mathrm{supp}\,(c)$ compact) is well defined and gives rise to an asymptotic series with a well behaved remainder term. Therefore,

$$\begin{aligned}\langle \varphi, c(x,D)\varphi\rangle &= \langle \psi, p^*(x,D)c(x,D)p(x,D)\psi\rangle \\ &= \langle \psi, \tilde{c}(x,D)\psi\rangle + \langle \psi, e\psi\rangle \ ,\end{aligned}$$

where e is an L^2-bounded remainder term. □

We only lack a reasonable criterion for $p(x,D)$ to be boundedly invertible in $L^2(\mathbb{R}^n)$. Without a symbol calculus we cannot simply make corrections to the natural choice $p^{-1}(x,D) \sim \exp(-b_0)(x,D)$. An easy criterion however, is to ask that $c_1(x,\xi)$ be small, and to use the resulting smallness of $b_0(x,D)$.

Theorem 23. *If $c_1(x,\xi)$ is sufficiently small, in the sense that for all $|\alpha|, |\beta| \le L$ the constants $C_{\alpha\beta}$ of the estimate*

$$|\partial_x^\alpha \partial_\xi^\beta c_1(x,\xi)| \le C_{\alpha\beta}\langle\xi\rangle^{1-|\beta|}\langle x\rangle^{-|\alpha|} \tag{71}$$

are sufficiently small, for some sufficiently large L, then the operator $p(x,D) = \exp(b_0)(x,D)$ is boundedly invertible in $L^2(\mathbb{R}^n)$.

Proof. Small constants in (71) imply that the $b_0(x,\xi)$ given by quadratures (13) and (22) is also small, which in turn means that the decomposition

$$p(x,\xi) = \exp(b_0(x,\xi)) = 1 + p_{(1)}(x,\xi)$$

gives the symbol $p_{(1)}(x,\xi) \in S_d^{0,0}(1,0)$, which is small. This results in an operator which is bounded on $L^2(\mathbb{R}^n)$, with small operator norm (see [6], section 4). Thus $p(x,D)$ is a small perturbation of the identity, and hence is clearly invertible. Notice that neither of the results Theorem 21 or Theorem 22 require any knowledge of the inverse in terms of pseudodifferential operators and their symbol properties, only that the inverse is bounded on $L^2(\mathbb{R}^n)$. □

§5. Mapping properties of $S_d^{0,0}(1,0)$

The transformation $p(x,D)$ of Section 4 involves symbols $p(x,\xi) \in S_d^{0,0}(1,0)$, and after transformation, the equation (59) involves coefficients with symbols in this class. This motivates the question of the boundedness properties of these pseudodifferential operators, on the classical Sobolev spaces and on the weighted Sobolev spaces that are used in previous sections of the paper. The two results below answer this basic question, and illustrate the role played by the special vector fields X_j defined in (17) and the geometric condition (21) on the support of such symbols.

Theorem 24. *Consider $p(x,\xi) \in S_d^{0,0}(1,0)$ which also satisfies the geometric condition (21) on its support. Then the operator $p(x,D)$ is bounded from $H^r(\mathbb{R}^n)$ to itself for all integers r.*

Proof. For $p(x,\xi) \in S_d^{0,0}(1,0)$ and $\varphi(x) \in \mathcal{S}$,

$$\begin{aligned}\partial_x p(x,D)\varphi =& \partial_x \int\int e^{i\xi(x-y)} p(x,\xi)\varphi(y)dyd\xi \\ =& \int\int e^{i\xi(x-y)} \big(\partial_x p(x,\xi)\varphi(y) + p(x,\xi)\partial_y\varphi(y)\big)dyd\xi \ .\end{aligned}$$

As $p(x,\xi) \in S_d^{0,0}(1,0)$, so also is $\partial_x p(x,\xi)$, and the support condition (21) is also shared. Hence, under the hypotheses of the theorem, the operator $p(x,D)$ maps $H^1(\mathbb{R}^n)$ into itself, and the rest follows by induction. □

The same question is natural when weighted norms are involved. Define the weighted Sobolev spaces $H^{r,s}(\mathbb{R}^n)$ with the norms

$$\|\psi(x)\|^2_{H^{r,s}} = \int |\langle x\rangle^s \langle \partial_x\rangle^r \psi(x)|^2 dx \ .$$

Theorem 25. *Given $p(x,\xi) \in S_d^{0,0}(1,0)$ which satisfies the support condition (21), the operator $p(x,D)$ is bounded from $H^{r,s}(\mathbb{R}^n)$ to itself. Furthermore, $p(x,\xi) \in S_d^{m,k}(1,0)$ satisfying (21) gives a pseudodifferential operator which maps $H^{r,s}(\mathbb{R}^n)$ to $H^{r-m,s-k}(\mathbb{R}^n)$.*

Proof. Starting from $p(x,\xi) \in S_d^{0,0}(1,0)$ and $\varphi(x) \in \mathcal{S}$, the multiplicative weights against $p(x,D)$ have the following result.

(73)

$$\begin{aligned}|x|^2 p(x,D)\varphi(x) &= |x|^2 \int\int e^{i\xi(x-y)} p(x,\xi)\varphi(y)dyd\xi \\ &= x\cdot \int\int (x-y)e^{i\xi(x-y)} p(x,\xi)\varphi(y)dyd\xi + x\cdot \int\int e^{i\xi(x-y)} p(x,\xi) y\varphi(y)dyd\xi \\ &= \int\int e^{i\xi(x-y)} ix\cdot\partial_\xi p(x,\xi)\varphi(y)dyd\xi + x\cdot \int\int e^{i\xi(x-y)} p(x,\xi)\varphi(y)dyd\xi \ .\end{aligned}$$

When $p(x,\xi) \in S_d^{0,0}(1,0)$, then $ix\cdot\partial_\xi p(x,\xi) \in S^{-1,1}(1,0)$ due to the property (18) with respect to the vector field X_3. Therefore, when $p(x,\xi)$ also satisfies the support condition (21), the Theorem 6 gives an estimate on $L^2(\mathbb{R}^n)$

$$\|\frac{|x|^2}{\langle x\rangle} p(x,D)\varphi\|_{L^2} \le C(\|\varphi(x)\|_{L^2} + \|x\varphi(x)\|_{L^2}) \ , \tag{74}$$

which implies that $p(x,D)$ is bounded from $H^{0,1}(\mathbb{R}^n)$ to itself. The rest of the statement of the theorem follows by induction. □

The final comment is on the necessity of the conditions (17),(18) and (21) for symbols of pseudodifferential operators, in order that they behave well on $L^2(\mathbb{R}^n)$. This is based on L. Hörmander's discussion in [8].

Theorem 26. *There are symbols $q(x,\xi) \in S^{0,0}(\rho,\delta)$ with $\delta < \rho$ such that $q(x,D)$ is not bounded on $L^2(\mathbb{R}^n)$.*

Proof. In reference [8], Corollary 5 gives examples of symbols $r(x,\xi) \in S^0_{\delta,\rho}$, the symbol classes introduced by Hörmander (that is,

$$|\partial_x^\alpha \partial_\xi^\beta r(x,\xi)| \le C_{\alpha\beta}(K)\langle\xi\rangle^{\rho|\alpha|-\delta|\beta|} ,$$

for $x \in K$ for any K compact) where $0 < \delta \le \rho < 1$ and $r(x,D)$ is not bounded from $L^2_{\mathrm{comp}}(\mathbb{R}^n)$ to $L^2_{\mathrm{loc}}(\mathbb{R}^n)$. Without loss of generality, we may take $\pi_x \mathrm{supp}\,(r) \subseteq K$, some compact set. Certainly $r(x,D)$ is not bounded on $L^2(\mathbb{R}^n)$, nor will be any extension of it outside of K. Set $q(x,\xi) = r(\xi,x)$ for $x \in \mathbb{R}^n$, $\xi \in K$, and extend $q(x,\xi)$ to be homogeneous of degree zero in ξ exterior to a large ball containing K, such that $q(x,\xi) \in S^{0,0}(\rho,\delta)$, the classes of Definition 5. Now $q(x,D)$ cannot be bounded on $L^2(\mathbb{R}^n)$, because otherwise $q^*(x,D)$ would be also, and then for any $\varphi \in L^2(\mathbb{R}^n)$, we would have

$$\|r(x,D)\varphi\|_{L^2} = \|q^*(x,D)\hat{\varphi}\|_{L^2} \le C\|\varphi\|_{L^2} .$$

□

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