Properties of microlocal smoothing for Schrödinger's equation

Walter Craig

CMLA, Ecole Normale Supérieure
94235 Cachan
France

and

Department of Mathematics
Brown University
Providence, Rhode Island 02912
USA

§1. Introduction: I want to talk about a number of recent results on the smoothness of solutions of the Schrödinger equation, which I find striking and quite intuitive to understand, despite the fact that in general the techniques of proof are somewhat technical. In these two lectures I will describe these results, and I will try to give a good picture of the heuristics which govern the smoothness properties of solutions, and as well describe some of the issues that one comes across in studying these questions. Toward the end of the lectures I will give a sketch of the ideas of the proof, and the techniques that are used in it. We will consider the following two equations:

(1) $$i\partial_t\psi = -12\Delta\psi x \in \mathbf{R}^n \quad \psi_0(x) = \psi(x,0) \in L^2(\mathbf{R}^n)$$

which is the usual free Schrödinger equation, and

(2) $$i\partial_t\psi = -12\sum_{j,\ell=1}^n \partial_{x_j} a^{j\ell}(x)\partial_{x_\ell}\psi + V(x)\psi x \in \mathbf{R}^n \quad \psi_0(x) = \psi(x,0) \in L^2(\mathbf{R}^n)$$

which is a more complicated Schrödinger equation with variable coefficients in a divergence form second order term, as well as lower order potential terms. Equation (1) has a well known explicit fundamental solution the free Schrödinger kernel, so in some sense we know all about its solutions. The equation (2) is more of a challenge, and will require us to work harder. I will start by describing some elementary properties of solutions of equation (1), and then go on to give their analogs for equation (2), to the extent that we know them. These properties of equation (1) are simple, but despite this I still think that they are remarkable, and certain of them are not sufficiently well known. The first theorem concerns solutions of equation (1).

Theorem 1: *Let $\psi_0(x) \in L^2(\mathbf{R}^n)$ be initial data for a solution $\psi(x,t)$ of equation (1).*
(i) Then for all $t \in \mathbf{R}$, $\psi(x,t) \in L^2(\mathbf{R}^n)$, with the same $L^2(\mathbf{R}^n)$ norm.

This is the simple and well known fact that evolution by solution of the Schrödinger equation is unitary on $L^2(\mathbf{R}^n)$, which is central to the interpretation of quantum mechanics. That is, measurements of a quantum particle are initially made with respect to the probability measure $dP_0(x) = |\psi_0(x)|^2 dx$, and at later time the measurements on the evolution of the particle are made with respect to the probability $dP_t(x) = |\psi(x,t)|^2 dx$. The result (i) is the fact that the evolution conserves probability. It seems then rather natural to impose conditions on the moments of the distribution $dP_0(x)$, as these are information about the location of the quantum paticle at time $t = 0$.

(ii) Suppose that additionally the probility $dP_0(x)$ has finite moments (for reasons of simplicity we will assume that all moments are finite, in order to avoid counting them). That is, we ask that

$$\forall k \text{ multiindices}, \quad \int |x^k \psi_0(x)|^2 dx < +\infty \ . \tag{3}$$

Then for all $t \neq 0$, $\psi(x,t) \in C^\infty$.

The purpose of this talk is to describe the analogous result for the equation (2). In the course of the description, I will give a proof of Theorem 1 as well.

§2. Results (for $V(x) = 0$): In order to start with the analysis of equation (2), I have to give the definition of several things.

Definition 1: (i) The *principal symbol* of the equation is the standard one, from the highest order terms of equation (2);

$$a(x,\xi) = 12 \sum_{j,\ell=1}^n a^{j\ell}(x)\xi_j\xi_\ell \ . \tag{4}$$

(ii) The *bicharacteristic flow* is the flow on the cotangent space $(x,\xi) \in T^*(\mathbf{R}^n)$ given by solutions of the Hamiltonian system

$$dxds = \partial_\xi a(x,\xi) d\xi ds = -\partial_x a(x,\xi) \ , \tag{5}$$

with the orbit originating at the point (x,ξ) denoted by $\varphi(s;x,\xi)$. Note particularly that the curves that are the orbits of the flow are parametrized by an auxiliary parameter s, which is not the time variable t.

(iii)(a) The classical definition of the *wave front set* of a distribution $f \in \mathcal{D}$ is given as follows. One defines the *singular support* $S(f)$ most easily by specifying what is not in it; a point $x_0 \notin S(f)$ if there is a cutoff function $\eta \in C_0^\infty$, with $\eta(x_0) = 1$, such that $(\eta f) \in C_0^\infty$. Using the duality between regularity in space and decay of the Fourier transform, we can alternately ask that

$$|\widehat{(\eta f)}(\xi)| \leq C_N \langle\xi\rangle^{-N}$$

for all $N \geq 0$, where we are using that $\langle x\rangle = (1 + |x|^2)^{1/2}$, notation common to this subject .

(iii)(b) The wave front set $WF(f)$ has a related definition. The point $(x_0, \xi^0) \notin WF(f)$ if there is a cutoff function $\eta \in C_0^\infty$ with $\eta(x_0) = 1$ and an open cone Γ with $\xi^0 \in \Gamma$ such that

$$|\widehat{(\eta f)}(\xi)| \leq C_N \langle\xi\rangle^{-N}$$

for all $\xi \in \Gamma$, for all $N \geq 0$.

The first theorem concerning the microlocal regularity of solutions of equation (2) is the following:

Theorem 2: (L. Boutet de Monvel (1974), R. Lascar (1977)) *For solutions of equation (2), the wave front set is an invariant set under the flow $\varphi(s;x,\xi)$ (with a slightly modified definition of the wave front set in $(x,t,\xi,\tau) \in \mathbf{R}^{2(n+1)}$, due to the inequality presented by having two spatial derivatives, compared to only one time derivative). This modification, which I do not give here, was called the quasi-homogeneous wave front set.*

This establishes a relation between the orbits of the flow of (3) and the singularities of the solution of (2), which states essentially that singularities travel with infinite velocity along the bicharacteristics of $a(x,\xi)$. However this statement confines our knowledge to each hyperplane $\{t = \text{constant}\}$, and it does not tell us how the singularities of the solutions will change in time. Continuing the items in our list,

(iv) Assume that the principal symbol is *nondegenerate*, which usually means elliptic

$$1C|\xi|^2 \leq a(x,\xi) \leq C|\xi|^2 \tag{6}$$

and *asymptotically flat*,

$$|\partial_x^\alpha(a^{j\ell}(x) - \delta^{j\ell})| \leq C\langle x\rangle^{-\tau(\alpha)}, \qquad \tau(\alpha) > |\alpha| + 1 \ . \tag{7}$$

Speaking of geometrical problems, the operator $-12\sum_{j,\ell=1}^n \partial_{x_j} a^{j\ell}(x)\partial_{x_\ell}$ is not quite the Laplace-Beltrami operator in general coordinates on an asymptotically flat manifold, for that requires $\det(a) = 1$. However all the analysis that we have in $L^2(\mathbf{R}^n, dx)$ carries over to the case of a Riemannian manifold with metric $ds^2 = \sum_{j\ell} g_{j\ell}(x)dx^j dx^\ell$, with the genuine Laplace-Beltrami operator

$$\Delta_g \psi(x) = 1\sqrt{\det(g)} \sum_{j,\ell=1}^n \partial_{x_j}(\sqrt{\det(g)}g^{j\ell}(x)\partial_{x_\ell})\psi(x)$$

where $g_{j\ell} = (g^{j\ell})^{-1}$, which is also self adjoint using the inner product on $L^2(\mathbf{R}^n, \sqrt{\det(g)}dx)$.

(v) One says that the point (x_0,ξ^0) is *not trapped forwards*, (respectively *backwards*) by the bicharacteristic flow φ of the symbol $a(x,\xi)$ if

$$|\varphi(s;x_0,\xi^0)| \longrightarrow \infty$$

as $s \longrightarrow +\infty$ (respectively, $s \longrightarrow -\infty$).

The theorem that we have proved in this subject concerns the time evolution of singularities in the solutions of (2), in contrast to Theorem 2.

Theorem 3 : (W. Craig, T. Kappeler and W. Strauss (1995)) *Suppose that the point (x_0,ξ^0) is not trapped backwards by the bicharacteristic flow φ of $a(x,\xi)$. Suppose that the moment condition (3) holds for the initial data $\psi_0(x)$. Then for any time $t > 0$,*

$$(x_0,\xi^0) \notin WF(\psi(x,t)) \ . \tag{8}$$

This is an entirely microlocal conclusion about the regularity of the solution of (2), however there is a global element as we must have information about the full backwards bicharacteristic through (x_0, ξ^0). There are also several global corollaries that follow essentially immediately from Theorem 3.

Corollary 4: *If $a(x,\xi)$ has no trapped bicharacteristics, then for initial data $\psi_0(x)$ satisfying (3), for all $t \neq 0$,*

$$WF(\psi(x,t)) = \emptyset \ ,$$

which is to say that $\psi(x,t) \in C^\infty$.

This latter statement is also a result of L. Kapitanski and Y. Safarov, who study the case of equation (2) when there are no trapped bicharacteristics, with quite different methods for their proof. Their approach is based on a relation between this problem and the classical problem of local time decay for solutions of the wave equation.

It is clear that this result also implies Theorem 1 (you might say it is a proof the hard way). From the Laplacian we have $a(x,\xi) = 12|\xi|^2$, and therefore Hamilton's canonical equations (5) are

$$dxds = \xi \ , \qquad d\xi ds = 0 \ .$$

The solutions are

$$x(s) = x_0 + s\xi^0 \ , \qquad \xi(s) = \xi^0 \ ,$$

which are straight line motion at constant velocity, and all bicharacteristics go to infinity in either direction. Thus Corollary 4 holds.

To give a more direct result for equation (1), the fundamental solution for the free problem is

$$S^0(x-y,t) = 1\sqrt{2\pi i t}^n e^{i|x-y|^2 2t} \ , \tag{9}$$

which is clearly an analytic function for $t \neq 0$. To prove a result related to Theorem 1, consider distributional initial data ψ_0 of compact support. The solution is then $S^0 * \psi_0$, which for any $t \neq 0$ is a compact sum of analytic functions, and is therefore itself analytic.

In general $a(x,\xi)$ may well have trapped bicharacteristics, so we cannot eliminate all singularities from the solution. We can however use Theorem 3 to confine the singularities to a subset of $T^*(\mathbf{R}^n)$ characterized by the dynamics. This is the intention of the next result.

Corollary 5: *Consider solutions $\psi(x,t)$ of equation (2), for time $t > 0$. Let R be the recurrent set of the bicharacteristic flow, and $M^u(R)$ the set of orbits which accumulate on R for $s \to -\infty$. Then*

$$WF(\psi(x,t)) \in R \cup M^u(R) \ . \tag{10}$$

Theorem 3 also allows us to discuss the fundamental solution $S(x,y,t)$ of the equation (2) in these terms. For this we have to consider the four variables $(x,\xi,y,\eta) \in T^*(\mathbf{R}^n) \times T^*(\mathbf{R}^n)$.

Corollary 6: *The point $(x_0,\xi^0,y_0,\eta^0) \in T^*(\mathbf{R}^n) \times T^*(\mathbf{R}^n)$ is not in the wave front set $WF(S(x,y,t) \subseteq T^*(\mathbf{R}^n) \times T^*(\mathbf{R}^n)$ for $t > 0$ if either*

(i) (x_0,ξ^0) is not trapped backwards, or

(ii) (y_0,η^0) is not trapped forwards

by the bicharacteristic flow φ of the principal symbol $a(x,\xi)$.

This result eliminates from the wave front set all points of the cotangent space which have the proper classical scattering behavior, however it is not a full characterization of the set on which the Schrödinger kernal is singular. There is a natural conjecture that one can make as to the full result for the problem, which I will state here. We are however not able with the present methods to prove this, and in fact a characterization of the evolution of $WF(S(x,y,t))$ promises to be a challenging problem. Any singularities must travel at infinite velocity, so points (x,y) at which $S(x,y,t)$ is singular must somehow be associated with noncompact subsets of the orbits of the bicharacteristic. The conjecture goes as follows: for $t>0$ the point $(x_0,\xi^0,y_0,\eta^0) \in WF(S(x,y,t))$ only if for any conic neighborhoods $(y_0,\eta^0) \in \Omega_1$ and $(x_0,\xi^0) \in \Omega_2$, there is a sequence $\{s_j\}_{j=1}^{\infty}$, with $s_j \rightarrow +\infty$, such that $\varphi(s_j;\Omega_1) \cap \Omega_2 \neq \emptyset$.

§3. Idea of the proof of Theorem 3: I want to concentrate on giving a good heuristic picture of the problem, before I talk about the actual analytic techniques that are employed in the proof. Restrict ourselves to the one dimensional case, and study the general (constant coefficient) equation

$$i\partial_t u = \omega(D)u \ , \quad x \in \mathbf{R} \tag{11}$$

where we are using the classical notation that $D = (1/i)\partial_x$. There are exponential solutions

$$u_\xi(x,t) = e^{i(\xi x - \omega(\xi)t)} \ ,$$

and for the general solution we can superpose these in a Fourier integral

$$u(x,t) = \int e^{i(\xi x - \omega(\xi)t)} \hat{u}_0 d\xi \ . \tag{12}$$

Lets make a solution which looks like a wave packet, by taking u_0 such that $\hat{u}_0 \in C_0^\infty$, in particular $\mathrm{supp}(\hat{u}_0) \subset\subset \mathbf{R}^n$, centered about some ξ^0. Solve the bicharacteristic equations

$$ddtx = \partial_\xi \omega \ , \qquad ddt\xi = -\partial_x \omega = 0 \ . \tag{13}$$

This gives solutions $x(t) = x_0 + t\partial_\xi\omega(\xi^0)$, and $\xi(t) = \xi_0$, which traverses a ray with velocity $\partial_\xi\omega(\xi^0)$ in the (x,t) plane. The following theorem relates this to the solution of (11).

Theorem 7: (the method of stationary phase) *In a cone away from the rays* $(x - t\partial_\xi\omega(\xi) =$ constant, $\xi \in$ supp $\hat{u}_0$, *the solution* $u(x,t)$ *decays faster than any polynomial.*

Proof: Suppose that we consider (x,t) such that for $\xi \in$ supp $\hat{u}_0$,

$$|xt - \partial_\xi\omega(\xi)| > R \ .$$

Then

$$u(x,t) = \int e^{i(\xi x - \omega(\xi)t)} \hat{u}_0(\xi) d\xi = \int 1 i(x - \partial_\xi\omega(\xi)t)\partial_\xi(e^{i(\xi x - \omega(\xi)t)})\hat{u}_0(\xi) d\xi = \int e^{i(\xi x - \omega(\xi)t)}\big(-\partial_\xi 1 i(x - \partial_\xi\omega(\xi)t)\big)\hat{u}_0(\xi) d\xi = \int e^{i(\xi x - \omega(\xi)t)}\big(-\partial_\xi 1 i(x - \partial_\xi\omega(\xi)t)\big)^N \hat{u}_0(\xi) d\xi \ .$$

for regular $\hat{u}_0$, for any integer $N \geq 0$. The denominator grows with magnitude $\langle Rt \rangle^N$, and the decay result will follow from this. ///

The quantity $\partial_\xi\omega$ is called the *group velocity*, a name given by Kelvin in his work on water waves. Using the picture of the evolution of a wave packet given by

Theorem 7, we can give a reason why the moments of the initial data are related to the smoothness of solutions for $t \neq 0$. Consider arbitrary data $u_0(x)$ of rapid decay, and cut its Fourier transform into pieces which each look like a wave packet solution, by using a partition of unity. That is

$$\hat{u}_0(\xi) = \sum_{k \in \mathbf{Z}} \hat{u}_k(\xi)$$

with each $\hat{u}_k(\xi) \in C_0^\infty(2Q_k)$, where Q_k is a cube of side one centered at the integer point k. The individual components $u_k(x,t)$ can be tracked (morally speaking) by Theorem 6, and are essentially confined to cones in the (x,t)-plane with slope near to $\partial_\xi \omega(k)$. To discuss the derives of the solution, isolate a bounded region K in x for $t \neq 0$; then the essential contributions of $u(x,t)$ in K are given by those components $u_k(x,t)$ for which the slope $\partial_\xi \omega(k)$ allows propagation from bounded regions of the initial data into our test region K. If the group velocity $\partial_\xi \omega(\xi)$ diverges as $|\xi| \to \infty$, only a finite number of the components are expected to essentially contribute to the solution in K, and therefore we can expect the solution to be smooth there. This is not a proof, but it is a compelling heuristic argument for the smoothing effects described above. Problems (11) for which $\partial_\xi \omega(\xi)$ diverges as $|\xi| \to \infty$ are called *dispersive*, and we expect that their singularities will travel with infinite velocity. The Schrödinger equation has $\omega(\xi) = 12|\xi|^2$, so that $\partial_\xi \omega(\xi) = \xi$, which is dispersive in the above sense.

I will now give a more precise description of the techniques used in the proof of Theorem 3, which are essentially microlocalized Sobolev estimates of the solution. Rewrite equation (2) as

$$i\partial_t \psi = A\psi \ , \tag{14}$$

where we assume that A is self adjoint. Then for any other operator B, solutions of (14) satisfy an identity

$$\partial_t \ \mathrm{re} \ \langle \psi, B\psi \rangle + \mathrm{re} \ \langle \psi, 1i[A,B]\psi \rangle = \mathrm{re} \ \langle \psi, (\partial_t B)\psi \rangle \ . \tag{15}$$

This identity gives us a small proposition, which includes the statement (i) of Theorem 1.

Proposition 8: *Any B which is time independent and commutes with A is preserved by the solutions of (2), that is,*

$$\partial_t \ \mathrm{re} \ \langle \psi, B\psi \rangle = 0 \ .$$

In particular, setting $B = I$, the L^2-norm of solutions are preserved.

We will make other choices of operator in the identity (15), in particular we will construct certain pseudodifferential operators for use in the proof. We define $B = b(x,D)$, where

$$b(x,D)\psi(x) = \int e^{i\xi\cdot(x-y)} b(x,\xi)\psi(y)dy \tag{16}$$

for 'symbol' $b(x,\xi) \in C^\infty(T^*(\mathbf{R}^n))$ chosen in a certain class of symbols for which this oscillatory integral is well behaved.

Definition 2: The usual definition of the class of *classical symbols* are those $b(x,\xi) \in C^\infty(T^*(\mathbf{R}^n))$ which satisfy

(17)(*i*) $\pi_x \mathrm{supp}\ (b) \subseteq K \subset\subset \mathbf{R}^n$ compactly supported

(17)(*ii*) $|\partial_x^\alpha \partial_\xi^\beta b(x,\xi)| \le C_{\alpha\beta} \langle \xi \rangle^{m-|\beta|}$.

L. Hörmander noticed that to retain most of the desirable symbol properties, it sufficed to replace (17)(ii) by

(17)(*iii*) $|\partial_x^\alpha \partial_\xi^\beta b(x,\xi)| \le C_{\alpha\beta} \langle \xi \rangle^{m-\delta|\beta|+\rho|\alpha|}$

for $0 \le \rho < \delta \le 1$. These classes of symbols are denoted $S^m(\delta,\rho)$. When $\rho = \delta < 1$ it is a critical case, which can be addressed to some extent by the theorem of Calderon and Vaillancourt.

The operator A can be written as a pseudodifferential operator, with symbol $a(x,\xi) + a_1(x,\xi)$, where there are both second and first order terms as A is in divergence form. The symbol $a_1(x,\xi) = i \sum_{j\ell} (\partial_{x_j} a^{j\ell}(x))\xi_\ell$. Composition of pseudodifferential operators, whose symbols are in suitable classes such as the above, is well defined in terms of the pseudodifferential calculus, and in fact the commutator in the identity (15) is described by

(18) $$1i[A, b(x,D)] = -\{a,b\}(x,D) + e \ ,$$

where the Poisson bracket is

(19)
$$\{a,b\}(x,\xi) = \sum_j (\partial_{\xi_j} a \, \partial_{x_j} b - \partial_{x_j} a \, \partial_{\xi_j} b)(x,\xi) = dds\Big|_{s=0} b(\varphi(s;x,\xi)) = X_a(b) \ .$$

The operator e is lower order, and X_a is the Hamiltonian vector field of the symbol a. We will use these operators in the identity (15), and if the relevant symbols are non-negative we can hope to obtain an energy-type estimate. Suppose that $b \in S^m$ of some symbol class, and count the orders of the operators in the identity (15). The error e will be of order m or possibly less, but the operator $\{a,b\}(x,D)$ is of order $m+1$, and is the most important contribution if the expression is to be useful. In fact, take the point of view that, given a symbol $c(x,\xi) \ge 0$ of order $m+1$, we will try to find $b(x,\xi)$ such that

(20) $$b(x,\xi) \ge 0 \ , \qquad \text{and} \qquad c(x,\xi) = -\{a,b\}(x,\xi) \ge 0 \ .$$

It is a fundamental question then whether pairs of symbols (b,c) exist satisfying the conditions (20).

Proposition 9: *Suppose that $c(x,\xi) \ge 0$, and that the point (x_0,ξ^0) is such that $c(x_0,\xi^0) > 0$ and that it is on a periodic bicharacteristic. Then there is no symbol $b(x,\xi)$ satisfying (20).*

Proof: The equation $\{a,b\} = -c$ is called a cohomological equation, and the regularity of the solution depends highly upon the recurrence properties of the flow φ. In the simple case of periodic orbits, if the symbol $b(x,\xi)$ did exist, then

$$0 < \int_0^P c(\varphi(s;x_0,\xi^0))ds = \int_0^P ddsb(\varphi(s;x_0,\xi^0))ds = \ 0 \ ,$$

which proves the result by contradiction. ///

However we can solve the cohomological equation for symbols $c(x,\xi) \geq 0$ by quadrature in the case that $\mathrm{supp}(c)$ has support only on bicharacteristics which are not trapped backwards. Indeed take $0 \leq c(x,\xi) \in S^{m+1}$ a classical symbol, with $\mathrm{supp}(c)$ in the set of orbits which are not trapped backwards, and set

$$b(x,\xi) = \int_0^{+\infty} c(\varphi(s;x,\xi))ds \ . \tag{21}$$

Then the support of $b(x,\xi)$ cannot be compact and there is a picture of the situation which is somewhat like this:

(figure 1)

Because the support of the symbols relevant to our work will not be compact, we need to keep track of their spatial behavior under differentiation as well as the behavior in the Fourier variables. The following theorem gives the behavior of the symbol $b(x,\xi)$ from (21).

Theorem 10: *Consider a classical symbol $c(x,\xi) \in S^{m+1}$, supported in the set of backwards nontrapping orbits (and suppose that $c(x,\xi) = 0$ for $|\xi| \leq 1$ to avoid troubles for small Fourier variables). Then in general all we can expect of $b(x,\xi)$ is the estimate*

$$|\partial_x^\alpha \partial_\xi^\beta b(x,\xi)| \leq C_{\alpha\beta} \langle\xi\rangle^{m-|\beta|} \langle x \rangle^{+|\beta|} \ . \tag{22}$$

That is, all we can expect from quadrature is a result which is in a very bad class of symbols, where no partial derivatives offset a lack of decay in spatial variables. We can call the class of such symbols $S^m(1,0)(0,1)$, where the first pair $(\delta_1, \rho_1) = (1,0)$ quantify the behavior in the Fourier variables, and the second pair $(\delta_2, \rho_2) = (0,1)$ describe their spatial behavior. The class $S^m(1,0)(0,1)$ does not form a symbol calculus, and in general may not even be bounded operators on $L^2(\mathbf{R}^n)$. However there is one extra property that is obeyed by symbols $b(x,\xi)$ constructed by the quadrature (21), which is related to their behavior under dilations in the fiber $\xi \in \mathbf{R}^n$. The vector field describing infinitessimal dilations is $\xi \cdot \partial_\xi$. Symbols defined by quadrature (21) satisfy the estimate

$$|(\xi \cdot \partial_\xi)^\gamma \partial_x^\alpha \partial_\xi^\beta b(x,\xi)| \leq C_{\alpha\beta\gamma} \langle\xi\rangle^{m-|\beta|} \langle x \rangle^{+|\beta|} \ . \tag{23}$$

With this estimate with respect to the vector field of dilations, the operators $b(x,D)$ are in fact better behaved than in general.

Theorem 11: *Suppose that $b(x,\xi)$ is a symbol such that*

$$|(\xi\cdot\partial_\xi)^\gamma \partial_x^\alpha b(x,\xi)| \le C_{\alpha\gamma} \ , \tag{24}$$

and suppose that there is a constant $R>0$ such that whenever $|x-y|>R$, and both $(x,\xi),(y,\xi)\in \mathrm{supp}\ (b)$, then

$$12|\xi|\langle x-y\rangle \le |(x-y)\cdot\xi| \ . \tag{25}$$

Then the operator $b(x,D)$ is bounded on $L^2(\mathbf{R}^n)$.

The symbols that one gets from quadrature (21) satisfy the estimate (24) and the support property (25) whenever the support of $c(x,\xi)$ is in a non-trapping region and is sufficiently small. From this we can see already an increment of additional regularity for the solutions of Schrödinger's equation (2); this is a microlocal version of what is sometimes called the 'local smoothing' property of dispersive equations. Let $c(x,\xi)$ be a classical symbol of order 1, supported in a sufficiently small conic neighborhood of a point (x_0,ξ^0) in the non-trapping region. Integrating the identity (15) over a time interval $[0,T]$, we obtain

(26)

$$\mathrm{re}\ \langle\psi, b(x,D)\psi\rangle(T) + \mathrm{re}\ \int_0^T \langle\psi, c(x,D)\psi\rangle(t)dt = \mathrm{re}\ \langle\psi_0, b(x,D)\psi_0\rangle + \mathrm{re}\ \int_0^T \langle\psi, (e(x,D) - 1i[a_1(x,D), b(x,D)])\psi\rangle(t)dt$$

All terms of this except the second are bounded by $\|\psi(x,t)\|^2_{L^2}$, and therefore, because of Theorem 1 (i), we have

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

The symbol of the operator $c(x,D)$ is nonnegative and is of order 1, therefore by Gårding's inequality, for any classical symbol $s(x,\xi)$ such that $0\le s^2(x,\xi)\le c(x,\xi)$,

$$\int_0^T \|s(x,D)\psi(t)\|^2 dt \le C(T)\|\psi_0\|^2_{l^2} \ . \tag{28}$$

Notice that $s(x,\xi)\in S^{1/2}$, therefore we have control of of a microlocal Sobolev estimate of 1/2-derivative of the solution, averaged in time, for any (x,ξ) in the region of phase space that is not trapped backwards by the bicharacteristic flow.

The full C^∞ result of Theorem 3 is given by an induction, which I will sketch here. Suppose that (x_0,ξ^0) is not trapped backwards, then we construct a conic neighborhood $\mathcal{E}^0_-$ of the backward bicharacteristic $\{\varphi(s;x_0,\xi^0) : s<0\}$, and a pair of symbols $b(x,\xi)\ge 0, c(x,\xi)\ge 0$, supported in $\mathcal{E}^0_-$ such that

$$c(x,\xi) = -\{a,b\}(x,\xi) \tag{29)(i}$$

(29)(*ii*)

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

These classes of symbols are called $S^{m,k}(1,0)(\delta,\rho)$. We have to manufacture such symbols so that $\rho<\delta$, and this we can do provided that $\delta+\rho>1$. When $\rho<\delta$ this symbol class gives a calculus of operators, which are used for microlocal bounds in the incoming regions of phase space. Applying the identity (15) to the pair

$t^p b(x,D), t^p c(x,D)$, for $b(x,\xi) \in S^{m,k}(1,0)(\delta,\rho)$, and $c(x,\xi) \in S^{m+1,k-1}(1,0)(\delta,\rho)$, the analog of (26) is
(30)

$$\mathrm{re}\ \langle \psi, t^p b(x,D)\psi\rangle(T) + \mathrm{re}\ \int_0^T \langle \psi, t^p c(x,D)\psi\rangle(t)dt = \mathrm{re}\ \langle \psi_0, t^p\big|_{t=0} b(x,D)\psi_0\rangle \quad + \mathrm{re}\ \int_0^T \langle \psi, (pt^{p-1}b(x,D) + t^p(e(x,D) - 1i[a_1(x,D), b(x,D)]))\psi\rangle(t)dt$$

For any $p > 0$, the first term of the RHS vanishes, and the estimate does not depend explicitely upon the initial data. We recognize in the remainder terms symbols in the class $t^{p-1}S^{m,k}(1,0)(\delta,\rho)$, and furthermore they are integrated in time over $[0,T]$. This is used in an induction, in which one starts with $k = K$ bounded orders of growth, and $m = 0$ demands of regularity. At the n-th induction step one takes $m = n, k = K - n$ and $p = n$. This will give the desired regularity result at any point which is not trapped backwards. When in addition the point (x_0, ξ^0) is also not trapped forwards, a similar induction gives the asymptotics of the growth of derivatives as $|x| \to \infty$. The geometry of this situation requires however that we use the worst case symbol class $S^{m,k}(1,0)(0,1)$, with inductive choices $m = n, k = -n - \epsilon$ and again $p = n$. Theorem 11 is used to control the error and to interpret the microlocal regularity of the solution from the resulting estimate.

§4. Results with a potential $V(x)$. The above is a discussion of the Schrödinger equation when no potential terms or other lower order terms are present. Let's now incorporate nonzero potentials in the problem, and see what effect this makes on the question of regularity. Consider potentials $V(x)$ for equation (2) which satisfy the growth conditions

$$|\partial_x^\alpha V(x)| \le C_\alpha \langle x\rangle^{p-|\alpha|}\ . \tag{31}$$

The power p controls the growth or decay of the potential at infinity. By the same techniques as above, we can prove that if $p < 1$ then the smoothness properties of the solutions with localized initial data ψ_0 are the same as if the potential were not present.

Theorem 12: *If $p < 1$ then then the conclusions of Theorem 3 continue to hold.*

The size of p is important to the problem, and for p sufficiently large the smoothing phenomenon cannot continue to hold. The critical power is $p = 2$, and indeed the quantum harmonic oscillator has explicit solutions which are instructive to discuss;

$$i\partial_t\psi = -12\Delta\psi + |x|^2 2\psi\ . \tag{32}$$

Theorem 13: *(i) Mehler's formula gives an explicit fundamental solution to (32).*
(33)

$$S^h(x,y,t) = 1\sqrt{2\pi i \sin(t)}^n e^{i\Phi}\ , \qquad \Phi(x,y,t) = 12(\cot(t)(|x|^2+|y|^2) - 2\csc(t)x\cdot y)\ .$$

The singularities of the quantum harmonic oscillator kernel occur at $x = y$ for $t = 0$, and then recur for every $t = n\pi, n \in \mathbf{Z}$. In the intervals between these times, the kernel is analytic, and at $t = 2n\pi$ the singularity is at $x = y$ again, while for $t = (2n+1)\pi$, the singularity is for $x = -y$ on the antipodal point of the potential well.

(ii) (A. Weinstein and S. Zelditch (1981)) For $a(x,\xi) = 12|\xi|^2$ and $V(x) = 12|x|^2 + v(x)$, where $v(x)$ is a Schwartz class function, then this same phenomenon of recurring of singularities occurs.

There has been recent work on this problem, with the principal symbol $a(x,\xi) = 12|\xi|^2$ of the Laplacian, and with various ranges of the growth parameter p.

Theorem 14: (K. Yajima, L. Kapitanski and I. Rodnienski)(1995) *Considering the Schrödinger equation*

$$i\partial_t\psi = -12\Delta\psi + V(x)\psi \ ; \tag{34}$$

with the potential satisfying (31) with any $p < 2$. The fundamental solution $S(x,y,t)$ is C^∞ for any $t \neq 0$.

This fills the gap left by Theorem 12 in the allowed values of p for which the smoothness of the fundamental solution is expected. The proofs of this theorem by K. Yajima is through a careful study of the trajectories of the classical Hamiltonian system with Hamiltonian $h(x,\xi) = 12|\xi|^2 + V(x)$, in the case of potentials satisfying (31) with $p < 2$. From this he constructs a parametrix for the problem in the form of those by H. Kitada and H. Kumano-go, which is valid in any finite interval $[-T,T]$. The proof by L. Kapitanski and I. Rodnienski uses completely different techniques, relying on certain specific operators which commute with the Schrödinger equation, modulo error terms which are lower order in derivatives as well as their spatial growth. The latter method depends very much on the fact that the operator A is the Laplacian, but the former construction may not depend so strongly on this, and it would be interesting to construct a proof of Theorem 3 and Theorem 12 for $p < 2$ by use of a parametrix.

Yajima also addresses the case $p > 2$ in his preprint, which gives the result that the fundamental solution lacks regularity.

Theorem 15: (K. Yajima (1995)) *Consider the problem (34) in one space dimension, and take $p > 2$. More precisely, ask that the potential $V(x) \in C^3(\mathbf{R})$, and outside of a bounded set ask that*

$$\partial_x^2 V(x) > 0 \ , \tag{35)(i}$$

$$x\partial_x V(x) > pV(x) > 0 \ , \tag{35)(ii}$$

and finally that for $j = 1, 2$ and 3,

$$\partial_x^j V(x) \partial_x^{j-1} V(x) = O\Big(1\langle x\rangle\Big) \ . \tag{35)(iii}$$

Then the fundamental solution $S(x,y,t)$ is a distribution kernel which is nowhere C^1.

I will finish with a description of the heuristics behind the results on potential terms, which depends upon the description of classical paths, and of course does not constitute a proof. Stay in one dimension for clarity, and consider the classical Hamiltonian systems associated with the problem (34). When $V(x) = 0$, the Hamiltonian is $h(x,\xi) = 12|\xi|^2$, the system is

$$ddtx = \partial_\xi h = \xi ddt\xi = -\partial_x h = 0 \tag{36}$$

and the flow $\varphi(t;x,\xi)$ in the phase plane is a shear flow $x(t) = x_0 + t\xi,\ \xi(t) = \xi^0$. The fundamental solution at $t = 0$ is a delta-function at $x = y$, which is schematically represented by marking the line which is its support in the phase plane. The evolution of the partial differential equation (34) can be imagined to be approximated at large Fourier transform variable by a distribution supported on the image of this line under the classical Hamiltonian flow $\varphi(t;x,\xi)$. The support of the delta-function and its evolution under the flow are pictured here.

(figure 2)

When $V(x) = 12|x|^2$, the classical harmonic oscillator, then $h(x,\xi) = 12|\xi|^2 + 12|x|^2$, and the flow in the phase plane is linear and consists of concentric circles about the origin, with every orbit periodic of the same period 2π. These orbits, and the evolution of the support of the initial delta-function are pictured in figure 3.

The feature of recurring singularities at $x = \pm y$ is accurately represented in the fact that the evolution of the line is vertical precisely at $x = \pm y$ at times $t = n\pi$.

(figure 3)

In the case $p < 2$, the interesting situation is for $V(x)$ growing at $|x| \to \infty$, in which case all orbits of classical solutions $\varphi(t; x, \xi)$ are periodic, but with period which becomes infinitely long as the energy $h(x, \xi) = 12|\xi|^2 + V(x)$ is taken to infinity. A rough sketch of the initial delta-function is as below. The feature that no interval of the configuration space $\{x \in \mathbf{R}\}$ is covered more than finitely often by the vertical projection of the curve, for $t \neq 0$ reflects accurately the fact that the Schrödinger kernel is smooth.

(figure 4)

Finally we can discuss the case of $p > 2$ in this way. For a potential such that $V(x)$ increases to infinity as $|x| \to \infty$ again all the classical orbits are periodic, but this time the period of the orbits decreases to zero as the energy $h(x, \xi) = 12|\xi|^2 + V(x)$ goes to infinity, corresponding to increasingly fast revolutions in phase space around the origin, for increasing radius. The projection of the image under $\varphi(t; x, \xi)$ of the support of the initial delta-function is now wrapped around the origin infinitely often, no matter which small time t is considered, and the projection of the resulting curve onto any interval of configuration space always has infinitely many components, which are unbounded in phase space. This is consistant with the conclusion of Theorem 15, and indeed gives an accurate heuristic argument for the result.

(figure 5)

Acknowledgements: These are lecture notes from a series of talks that were given at the Institute of Mathematical Sciences in Madras, contributing to the Workshop on Schrödinger operators which was held on 4 - 14 December 1995. I would like to thank the Institute of Mathematical Sciences and especially Krishna Maddaly for organization and support of this workshop, and for their kind hospitality during my stay. My travel to India was supported by the National Science Foundation under the International Programs Grant *INT - 95 28154*.