Singularities of Schrödinger's equation and recurrent bicharacteristic flow

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This note is concerned with solutions of the time dependent Schrödinger equation

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

with $x \in \mathbf{R}^n$. The Schrödinger kernel $S(x, y, t)$ is a distribution on $\mathbf{R}^n_x \times \mathbf{R}^n_y \times \mathbf{R}_t$, and we are interested in a microlocal description of its singularities. It is usual to consider modifications of equation (1) with an additional potential term or with first order terms which arise when describing the effects of an external potential or an electro-magnetic field. The situation for (1) is however already interesting, and for the most part we will focus on it. Much of the analysis carries through in the more general setting of a complete Riemannian manifold whose non-compact ends are endowed with scattering metrics, again we will mostly remain with the case at hand. The discussion below consists of excerpts from two seminar talks given at the MSRI in Berkeley on 23 October and the Fields Institute in Toronto on 28 October 1997.

The free euclidian case corresponds to $a^{j\ell} = \delta^{j\ell}$, for which

$$i\partial_t\psi = -\tfrac{1}{2}\Delta\psi \ , \tag{2}$$

and the Schrödinger kernel is explicitely

$$S^0(x-y,t) = \frac{1}{\sqrt{2\pi i t}^{\,n}} e^{\frac{i|x-y|^2}{2t}} \ . \tag{3}$$

From this expression we observe a number of self evident facts.

Proposition 1: *Given $\psi(x,t)$ a solution of (2) with $\psi_0(x) \in L^2(\mathbf{R}^n)$, define the probability distributions*

$$dP_t(x) = |\psi(x,t)|^2 dx \ .$$

(i) Schrödinger evolution conserves probability,

$$\int_{\mathbf{R}^n} dP_t(x) = \int_{\mathbf{R}^n} dP_0(x) \ .$$

(ii) If $dP_0(x)$ possesses all of its moments,

$$\int_{\mathbf{R}^n} |x^k\psi_0(x)|^2 dx < +\infty \ , \tag{4}$$

then for all $t \neq 0$, the solution $\psi(x,t)$ is C^∞.
(iii) Given a distribution $\psi_0 \in \mathcal{D}'$ for initial data which possesses all of its moments, then the solution $\psi(x,t)$ is again C^∞ for all $t \neq 0$.

An interpretation of this is that all singularities in the data are carried to infinity instantly by the solution operator for equation (2). To understand the analogous phenomenon in the more general setting of equation (1), consider the principal symbol $a(x,\xi) = \frac{1}{2}\sum_{j,\ell} a^{j\ell}(x)\,\xi_j\xi_\ell$, whose bicharacteristic flow on $T^*(\mathbf{R}^n)$ we denote by $\varphi_s(x,\xi)$. The first connection between singularities and the bicharacteristic flow was given by L. Boutet de Monvel [1] and R. Lascar [8], who proved that for solutions of (1), the (appropriate quasi-homogeneous) wave front set $WF_Q(\psi(x,t)) \subseteq T^*(\mathbf{R}^n_x \times \mathbf{R}_t)$ is invariant under the flow $\Phi_s(x,\xi,t,\tau) = (\varphi_s(x,\xi),t,\tau)$. The proof of this is closely related to L. Hörmander's classical results [6] on the propagation of singularities for hyperbolic equations. In our case (1) the implication is that singularities must propagate with infinite velocity along bicharacteristics, and that the wave front set of solutions is a 'horizontal' set in space-time. These results do not however predict the evolution of singularities in time t. For illustration, the wave front set of the free Schrödinger kernel $S^0(x,t)$ is precisely $WF(S^0(x,t)) = \{(x,\xi,t,\tau) : t = \tau = 0, \xi/|\xi| = \pm x/|x|\}$, the set of radial lines eminating from and returning to the origin at $t = 0$.

An improvement to this result can be made under a hypothesis of nonrecurrence of the bicharacteristic flow. We consider elliptic operators $\sum_{j\ell} \partial_{x_j} a^{j\ell}(x) \partial_{x_\ell}$ such that

$$|\partial_x^\alpha (a^{j\ell}(x) - \delta^{j\ell})| \le \frac{C_\alpha}{\langle x \rangle^{|\alpha|+1+\epsilon}} .$$

In case we have normalized $\det(a) = 1$ these are Laplace-Beltrami operators for the asymptotically flat metric $ds^2 = \sum_{j\ell} a_{j\ell}(x) dx^j dx^\ell$.

Theorem 2: *(W. Craig, T. Kappeler & W. Strauss [3]) Suppose that $(x_0, \xi^0) \in T^*(\mathbf{R}^n)$ is not trapped backwards, that is, it is carried to infinity by the bicharacteristic flow $\varphi(s; x, \xi)$ as $s \to -\infty$. Given data $\psi_0(x)$ which satisfies the moment condition (4), then for all $t > 0$,*

$$(x_0, \xi^0) \notin WF(\psi(x,t)) . \tag{5}$$

In the nonelliptic case there are results of a similar nature which appear in [3], and there are further results in recent unpublished work by C. Kenig, G. Ponce, C. Rolvung, and L. Vega. The moment condition is of course overly strong, one may replace it with a condition on the moments of ψ_0 appropriately microlocalized near the past of the bicharacteristic through (x_0, ξ^0).

A number of global corollaries follow directly from this statement. Define the *recurrent set* of the bicharacteristic flow to be $R = \{(x,\xi) \in T^*(\mathbf{R}^n) \backslash \{0\} : \varphi(s : x, \xi)$ is bounded for all $s \in \mathbf{R}\}$, and let $M^u(R) = \{(x,\xi) : \varphi(s : x,\xi)$ is bounded for all $s \le 0\} \backslash R$.

Corollary 3: *(i) Whenever $\psi_0(x)$ satisfies (4), then for all $t > 0$*

$$WF(\psi(x,t)) \subseteq R \cup M^u(R) .$$

(ii) Consider the Schrödinger kernel $S(x,y,t)$. Whenever either (x_0,ξ^0) is not trapped backwards, or else (y_0,η^0) is not trapped forwards by the bicharacteristic flow $\varphi(s;x,\xi)$, then for all $t>0$

$$(x_0,\xi^0,y_0,\eta^0) \notin WF(S(x,y,t)) \ . \tag{6}$$

Recently J. Wunsch [9] has substantially improved this theorem and its corollaries in the setting of scattering metrics at infinity. However it is evident that the picture of the singularities of the Schrödinger kernel is far from complete, and that it is intimately connected with the recurrence properties of the flow $\varphi(s)$. Because of infinite propagation speed, it is not sufficient to connect a point $(y_0,\eta^0) \in T^*(\mathbf{R}^n)$ with $(x_0,\xi^0) \in T^*(\mathbf{R}^n)$ with a bicharacteristic, in order that $(x_0,\xi^0,y_0,\eta^0) \in WF(S)$. Rather we must have a situation in which the bicharacteristic flow of neighborhoods of (y_0,η^0) is recurrent at (x_0,ξ^0). The following conjecture is therefore compelling.

Conjecture 4: *For $t>0$ the point (x_0,ξ^0,y_0,η^0) is in $WF(S(x,y,t))$ only if, for any conic neighborhoods Ω_1,Ω_2, with $(x_0,\xi^0)\in\Omega_1$ and $(y_0,\eta^0)\in\Omega_2$, then there is a sequence of times $s_j\to+\infty$ such that*

$$\varphi(s_j;\Omega_2)\cap\Omega_1 \neq \emptyset \ .$$

Aside from several examples which are compatible with this statement and a few results in special cases, this question remains open.

The simplest example of a recurrent situation is to pose equation (2) in one dimension on the circle S^1. The Schrödinger kernel is again explicit

$$S^{per}(x-y,t) = \sum_{k\in\mathbf{Z}} \frac{1}{2\pi} e^{ik^2t/2} e^{ik(x-y)} \ , \tag{7}$$

yet it is nonetheless interesting. At rational times $t/2\pi = p/q$ (in lowest terms) S^{per} decomposes into a linear combination of δ-functions, supported at translates of the q^{th} roots of unity. Note that $WF(S^{per}) \subset T^*(S^1_x)\times T^*(S^1_y)$ is thus intermittent, while $WF_Q(S^{per}) \subseteq T^*(S^1_x\times S^1_y\times\mathbf{R}_t)$ is not, and is larger. For $2\pi t\in\mathbf{R}\backslash\mathbf{Q}$ the regularity of S^{per} is worse; it is not even a measure [5], and in fact its regularity is related to the diophantine properties of $t/2\pi$ [7]. In any case, all

$(y, \eta) \in T^*(S^1)$ are recurrent to all $(x, \xi) \in T^*(S^1)$, supporting the above conjecture.

A next most simple example is a manifold which is asymptotically hyperbolic, constructed from the upper half space, $M = \mathbf{H}^d \backslash \Gamma$, where Γ is generated by one hyperbolic element. When the dimension d is odd the heat kernel $H(x, y, t)$ has an explicit description in geometrical terms, and one may simply continue it for complex time to obtain the Schrödinger kernel $S(x, y, t) = H(x, y, it)$. The manifold M has one simple closed geodesic. Inspecting $S(x, y, t)$ on this periodic geodesic it is easy to see that it possesses a singularity, indeed the same singularity as for the circle S^1 of the previous example.

As a final remark, there is a theorem of S. Doi [4] which addresses the recurrence of bicharacteristics and relates it to the local smoothing property of solutions of Schrödinger's equation. His statement is essentially that a microlocal smoothing property of order 1/2 holds on bicharacteristics which are not trapped, however it cannot hold for any conic neighborhood Ω of a point (x_0, ξ^0) at which the bicharacteristic flow is recurrent.

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