# NICE MINICOURSE: WKB SOLUTIONS AND PROPAGATION OF SINGULARITIES

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We consider the Helmholtz equation with variable sound speed

$$(-\Delta + k^2 V(x))u = f_0$$

and do a semiclassical rescaling to turn this equation into

$$(-h^2\Delta + V(x))u = f \tag{1}$$

with $f = k^{-2} f_0 = h^2 f_0$. This is already quite interesting with $f = 0$ on a compact domain (with boundary conditions), especially if we make the modification to

$$(-h^2\Delta + V(x) - E)u = 0, \tag{2}$$

which is the (stationary) Schrödinger equation. Note that we always consider a *family* of solutions, hence for each $h \in (0,1)$ (or for a discrete sequence of values of this parameter) we have a discrete set of $E = E_j(h)$ for which this inhomogeneous equation should have a solution (we appeal here to standard elliptic regularity theory). Another very interesting special case: consider (1) with $f = \delta_{x_0}$ (i.e. we seek a fundamental solution). Or take $f$ to have small support, and study solutions to homogeneous equation away from support of $f$. Or homogeneous solution with data "at infinity" (*scattering*: see Martin Vogel).

Semiclassical microlocal analysis has two faces: it allows us both to *construct* solutions, or approximate solutions, to PDE problems like (2); and it allows us to analyze the asymptotic regularity of solutions to these equations via *energy estimates*. The former approach has the virtue of being more explicit: we produce a *formula* for the solution. The latter has the virtue of being more flexible and adaptable, as well as dealing more directly with $L^2$ or Sobolev estimates which may or may not be apparent from a complicated formula. These lectures will deal with both approaches in turn. The first, on WKB methods, will just touch the tip of the iceberg of the constructive ("parametrix") methods that make up the modern theory of Lagrangian distributions, a.k.a. Fourier integral operators. The second will deal with the analysis of semiclassical wavefront sets and their close relative, microlocal defect measure; we will prove a propagation of singularities result based just on $L^2$ estimates rather than on knowing a solution explicitly—this is really a way of thinking about energy estimates for our equation in phase space.

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# 1. Lecture 1: WKB

Let's discuss a nice way to try to locally construct solutions to[1]

$$(-h^2\Delta + V(x))u = 0. \tag{3}$$

Seek $h$-dependent family of solutions $u = u(x; h)$, but in notation we often suppress the $h$.

Trivial example

$$(-h^2\partial_x^2 - E)u = 0 \text{ on } \mathbb{R} :$$

solutions

$$e^{\pm i\sqrt{E}x/h}.$$

Note rapid oscillation as $h \downarrow 0$; frequency is $\sqrt{E}/h$. More generally try an Ansatz

$$u(x; h) = a(x; h)e^{i\phi(x)/h}. \tag{4}$$

Here $a$ should depends on $(x, h) \in \mathbb{R}^n \times [0, 1)$ and will ultimately have (formal) asymptotic expansion in powers of $h$ with smooth coefficients:

$$a(x; h) \sim a_0(x) + ha_1(x) + \dots,\ a_j(x) \in \mathcal{C}^\infty(\mathbb{R}^n), \tag{5}$$

and $\phi$ is independent of $h$.[2] So asymptotic oscillation *exactly* known and amplitude can be Borel summed to be smooth in $h$. We will settle for approximate solutions (say mod $O(h^\infty)$. This is called the WKB (Wentzel–Kramers–Brillouin) method (or maybe BKW; vive la France). Or the method of geometric optics.

Try Ansatz (4) in (3). We get, grouping terms in which the derivatives fall on $a$ and $e^{i\phi/h}$ and dropping an overall factor of $e^{i\phi/h}$,

$$-h^2\Delta a + Va - 2hi\nabla\phi \cdot \nabla a + |\nabla\phi|^2 a - hi\Delta\phi a = 0. \tag{6}$$

The largest terms here, in terms of powers of $h$, are the two $O(1)$ terms

$$|\nabla\phi(x)|^2 a + V(x)a; \tag{7}$$

thus, unless $a = O(h)$ (which would be a problem for e.g. having $L^2$ normalized solutions) the only way to solve our equation is to take

$$|\nabla\phi(x)|^2 + V(x) = 0. \tag{8}$$

This is called the *eikonal equation* (or Hamilton–Jacobi equation). How might we solve it? This is an interesting (and long) story, and to make the logical flow clear, we'll do this in a separate subsection.

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[1] You might want to consider a spectral parameter $E$, but we can absorb it into $V$ for these purposes. It's useful to keep in mind, in order to have useful examples, that $V$ does not have fixed sign.

[2] We could of course take $\phi$ also to be a power series in $h$ but the exponential of $O(h)$ terms can just be lumped back into $a$ without loss of generality.

1.1. **Eikonal equation.** Idea: seek not $\phi$ but rather the graph $d\phi$ (so recover $\phi$ up to constant). Thus, set

$$\Lambda = \{(x, d\phi(x) \colon x \in \mathbb{R}^n\} \subset T^*\mathbb{R}^n$$

The notation $d\phi = \sum(\partial\phi/\partial x_j)dx^j$ is for our purposes just a more invariant way to think of $\nabla\phi$. $T^*\mathbb{R}^n$ denotes the *cotangent bundle*, which you can just take to be $\mathbb{R}^n_x \times \mathbb{R}^n_\xi$. In this notation, $\Lambda$ lies inside the *energy surface*

$$|\xi|^2 + V(x) = 0$$

But this energy surface has codimension 1 and $\Lambda$ has codimension $n$ (so much smaller in general). The submanifold $\Lambda$ is defined by $\xi = \nabla\phi(x)$ of course.

Now consider the vector field[3]

$$\mathsf{H} \equiv 2\xi \cdot \partial_x - \nabla V(x) \cdot \partial_\xi$$

on $T^*\mathbb{R}^n$. Since $\Lambda$ is defined by $\xi_j - \partial_j\phi(x) = 0$ for $j = 1, \dots, n$, applying this vector field to the $j$'th defining function gives

$$-2\sum_i \xi_i \partial_{x_i}\partial_{x_j}\phi(x) - \partial_j V(x).$$

Since

$$\xi_i = \partial_{x_i}\phi$$

on $\Lambda$, this yields by the chain rule just

$$-\partial_{x_j}|\nabla\phi|^2 - \partial_j V(x),$$

and this vanishes on $\Lambda$!

Where did this crazy vector field come from? It's the *Hamilton* vector field, the generator of classical dynamics via the equations for its flow, which read simply

$$\dot{x} = 2\xi_j, \quad \dot{\xi} = -\nabla V.$$

Plugging one into the other gives the second order equation

$$\ddot{x} = -2\nabla V,$$

which is simply Newton's law in the potential $V$, up to a pesky factor of 2 that we haven't bothered with.[4] The equations for $(x, \xi)$ jointly are *Hamilton's equations of motion*, with $\xi = (1/2)\dot{x}$ representing the momentum along the classical flow.

[3]We will use the geometers' notation for vector fields that identifies a vector field with the directional derivative along it; hence in $\mathbb{R}^d$ with coordinates $y_1, \dots, y_d$, instead of writing a vector as

$$\mathbf{v} = \begin{pmatrix} v_1 \\ \vdots \\ v_d \end{pmatrix},$$

we identify it with the first order operators $\sum v_j\partial_{y_j}$ or $\mathbf{v} \cdot \nabla$.

[4]The operator really ought to have been $-(1/2)h^2\Delta + V$ to make this work out.

We've thus showed

**Proposition 1.** *If $\phi$ is a smooth solution to the eikonal equation* (8) *then the Hamilton vector field* $\mathsf{H}$ *is tangent to* $\Lambda = \operatorname{graph}(d\phi)$.

(This is the basic fact of what's called *Hamilton–Jacobi theory.*) Thus integral curves of $\mathsf{H}$ that start in $\Lambda$ stay in $\Lambda$.[5]

Now secretly, (3) is a *hyperbolic* equation in the sense of semiclassical asymptotics. (Stuff propagates.) So we'll try to solve from one side of a hypersurface:[6] split $x = (x_1, x')$ and specify $a, \phi$ for $x_1 \leq 0$; we'll try to extend the solution across the hypersurface by solving for $x_1 > 0$. The above proposition allows us to try to extend our solution for $\phi$ as long as the flow direction of $\mathsf{H}$ is transverse to $x_1 = 0$, i.e. $\xi_1 = \partial_{x_1}\phi \neq 0$ at the points in question. We are given

$$\Lambda\big|_{x_1=0} \equiv \Lambda_0,$$

Suppose WLOG that $\partial_{x_1}\phi > 0$ along $x_1 = 0$ so that $\mathsf{H}$ points to the right. We simply now define, over $x_1 > 0$

$$\Lambda = \{\exp_{t\mathsf{H}}(\rho) : \rho \in \Lambda_0,\ t < \epsilon\}$$

**Proposition 2.** *For $\epsilon > 0$ sufficiently small, this $\Lambda$ continues to be a manifold that projects diffeomorphically to $\mathbb{R}^n_x$; there exists a smooth $\phi$ such that*

$$\Lambda = \operatorname{graph}(d\phi)$$

*and $\phi$ solves* (8).

*Exercise* 1. Prove this! Note that you'll have to prove that when we write $\xi = \Xi(x)$, exhibiting $\Lambda$ as a graph over the $x$ variables, we have

$$d(\Xi(x) \cdot dx) = 0,$$

so that $\Xi(x) \cdot dx = d\phi$ for some $\phi$. (If you prefer, this is just the compability condition $\partial\Xi_i/\partial x_j = \partial\Xi_j/\partial x_i$.)[7] You'll also have to check that the resulting $\phi$, provided it makes sense, satisfies (8). For this, it's important to note that $\mathsf{H}(\xi^2 + V) = 0$.

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[5]You're getting the abbreviated version here, of course. The language and methods of *symplectic geometry* make this all less crazy. $\Lambda$ is a *Lagrangian submanifold* of the *symplectic manifold* $T^*\mathbb{R}^n$ lying inside the set where $p = |\xi|^2 + V$ vanishes. It's then an important (and easy) general theorem that the Hamilton vector field of $p$ (generating the dynamics of $p$ as a classical Hamiltonian) is tangent to $\Lambda$.

[6]Really it would be better to think about solving the Cauchy problem starting with data on the hypersurface, but we'll leave this for you as an exercise as you have to think about what the right data should be.

[7]A hint to the hint, since this is a substantial problem, is that if you know some geometry of differential forms, you can check that the time derivative along the $\mathsf{H}$-flow of $\sum d\xi_j \wedge dx_j$ restricted to $\Lambda$ is zero, by using Cartan's formula, and then to note that the vanishing of this quantity is locally equivalent to $\Lambda$ projecting diffeomorphically to the base variables $x$, by the Poincaré lemma.

*Exercise* 2. Do this construction explicitly for $V = -E$ a constant and with $\phi = \alpha \cdot x$.

Note that we cannot expect to continue this process forever—it's only local. The trouble is that eventually $\Lambda$ may fold over and cease to continue to be a graph over $\mathbb{R}^n_x$. And then it gets really fun: this is the general theory of Lagrangian distributions, a.k.a. FIOs (see, e.g., Hörmander FIO1).

1.2. **Transport equations.** Finally, let's return to our proposal for solving the Helmholtz equation. All that work solving (8), and we've only solved our equation mod $O(h)$ terms. Let's now return to the equation (6), which now with the eikonal equation satisfied reads (after dropping an overall factor of $h$)

$$-h\Delta a - 2i\nabla\phi \cdot \nabla a - i\Delta\phi a = 0. \tag{9}$$

Since there are two different powers of $h$ involved here, we'll necessarily have to deal with it (in general) by solving iteratively as a formal power series in $h$. Recalling the expansion (5), we now group like powers of $h$. Here is the $h^0$ term (after taking out a constant factor):

$$\nabla\phi \cdot \nabla a_0 + \frac{1}{2}(\Delta\phi)a_0 = 0.$$

This one is easy to solve by integration: Remember that by assumption, $\partial_{x_1}\phi \neq 0$ at $x_1 = 0$, so we can think of this as an ODE along the integral curves of the vector field $\nabla\phi$, which are transverse to $x_1 = 0$.

*Exercise* 3. Solve the inital value problem for this with data at $x_1 = 0$ in terms of the flow of the vector field $\nabla\phi$ by using an integrating factor.

How about the next one? The $h^1$ equation reads

$$-\Delta a_0 - 2i\nabla\phi \cdot \nabla a_1 - i\Delta\phi a_0 = 0.$$

Rewriting this as

$$\nabla\phi \cdot \nabla a_1 + \frac{1}{2}(\Delta\phi)a_1 = \frac{i}{2}\Delta a_0$$

we note that it is again an equation, this time for, $a_1$ along the vector field $\nabla\phi$, but this time with nonvanishing RHS determined by our previous step; again we can solve by integration! (A so-called *transport equation.*)

Subsequent equations are of the same form, and can be solved by integration along the v.f. $\nabla\phi$ in the same manner.

1.3. **Taking stock.** Proceeding in this manner, we can for any $N$ find $a_0, \dots, a_N$ so that if $\tilde{a}_N = a_0 + ha_1 + \cdots + h^N a_N$ then

$$(-h^2\Delta + V)(\tilde{a}_N e^{i\phi/h}) = O(h^{N+2}).$$

If we prefer, we can in fact *Borel sum* to $a \sim a_0 + ha_1 + \dots$ to solve the very accurate "quasimode equation"

$$(-h^2\Delta + V)(ae^{i\phi/h}) = O(h^\infty).$$

*Exercise* 4. Understand Borel summation, and why it's related to the calculus lemma that any sequence of numbers at all are the Taylor coefficients of some smooth function on $\mathbb{R}$.

This is pretty good, but it's as far as we're going to get without further input. How can we get rid of an $O(h^\infty)$ error? If we have some kind of estimate for the inverse of $(-h^2\Delta+V)$ then maybe we can do this, but such an estimate isn't always available. See Martin's lecture.

Takeaway for next time: remember that $\Lambda$, the graph of $d\phi$, gets propagated in $T^*\mathbb{R}^n$ along the flow of $\mathsf{H}$, a.k.a. classical trajectories in phase space. The support of $a$ comes along for the ride, since it propagates along $\nabla\phi\cdot\partial_x = \xi\cdot\partial_x$ on $\Lambda$; this is the expression for $\mathsf{H}$ when we use $x$ as coordinates for $\Lambda$.

## 2. Lectures 2–10: Propagation of singularities

Let us try to use our knowledge of PsiDOs to understand how solutions to the Helmholtz equation (1) may *concentrate*. Remember that last time we managed to produce (approximate) solutions we associated to a submanifold of phase space graph $d\phi$ where $\phi$ satisfied the eikonal equation. Keep this class of examples in the back of your mind for this second lecture.

A first approximation to the question of concentration is: as $h \downarrow 0$, for which $x$ is $u(x;h)$ not decaying to zero? But it turns out to be very productive to ask for more: we will identify where $u$ lives in *phase space*, which is to say where is it localized in $x$, and to what degree is it asymptotically oscillating like the solutions that we considered yesterday, which look more or less like $e^{i\xi\cdot x/h}$? We'd like to recover a sensible $\xi$, even if $u(x;h)$ did not arise as an explicit WKB solution.

I offer you two options for making these measurements, each with their own virtues and applications. I'll focus on the latter (defect measure).

### 2.1. **Wavefront set.**

(Recap of Melissa's lecture.) As always, $u$ depends on both $x$ and $h$ with the (crucial!) latter dependence suppressed in notation.

*Definition* 3. Let $(x_0,\xi_0)\in T^*\mathbb{R}^n$. Then $(x,\xi)\notin \mathrm{WF}_h(u)$ if there is $a(x,\xi)$ with $a(x_0,\xi_0)\neq 0$, and so that

$$\mathrm{Op}_h(a)u = O(h^\infty).$$

We have thus defined the *complement* of the wavefront set: this point is *not* in it if we can *localize* in phase space by applying a PsiDO that's nontrivial at this point, and we get something trivial ($O(h^\infty)$) out. For purposes of comparison, you might like to define $\operatorname{ess-supp} u$, the *essential support*, by $x_0\notin \operatorname{ess-supp} u$ if there exists $\psi\in\mathcal{C}^\infty(\mathbb{R}^n)$, $\psi(x_0)\neq 0$, $\psi u = O(h^\infty)$. This just measures where $u$ is nontrivial in *position*, while our definition above does more (it gets momentum too).

*Exercise* 5. Let $u$ have compact support. Show that $\operatorname{ess-supp} u = \emptyset$ iff $u = O(h^\infty)$ globally.

**Proposition 4.** *Let $\pi$ denote the projection $T^*\mathbb{R}^n \to \mathbb{R}^n$. Then*[8] $\pi(\mathrm{WF}_h\, u) = \text{ess-supp}\, u$.

So in particular there is no WF in the fiber over a single point iff $u = O(h^\infty)$ near that point.

Let's take the special case of testing by $A = \mathrm{Op}_h(\phi(x)\psi(\xi))^*$ where $\phi$ and $\psi$ localize near $x = x_0$ resp. $\xi = \xi_0$. This gives

$$Au = \mathcal{F}_h^{-1}\psi(\xi)\mathcal{F}_h(\phi(x)u),$$

with $\mathcal{F}_h$ the semiclassical FT.

*Exercise* 6. There exists $A$ as above with $Au = O(h^\infty)$ iff $\mathcal{F}_h(\phi(x)u) = O(h^\infty)$ in a nbd. of $\xi_0$.

This special family of operators in fact turns out to be general enough to use for testing for WF, and we obtain the following handy local definition:

**Proposition 5.** *A point $(x_0, \xi_0)$ is not in $\mathrm{WF}_h\, u$ iff there is a cutoff $\phi$ near $x_0$ so that*

$$\mathcal{F}_h(\phi u) = O(h^\infty) \text{ in a neighborhood of } \xi_0.$$

*Exercise* 7. Compute $\mathrm{WF}_h\, e^{i\alpha x/h}$, $\mathrm{WF}_h\, a(x)$ (with $a$ smooth and independent of $h$).

**Proposition 6.** $\mathrm{WF}_h\, u$ *is coordinate invariant as a subset of $T^*\mathbb{R}^n$.*

*Exercise* 8. Understand what this means, if you've never grappled with $T^*\mathbb{R}^n$ before.

*Exercise* 9. Assume that $\phi$ has no critical points, and compute

$$\mathrm{WF}_h\, e^{i\phi(x)/h}$$

Hint: change coordinates locally to make $\phi$ linear! Alternatively, think about the fact that $u = e^{i\phi(x)/h}$ satisfies the equations

$$(hD_j - \partial_j\phi)u = 0.$$

**Theorem 7.** *Let $A \in \Psi_h(\mathbb{R}^n)$. Then*

$$\mathrm{WF}_h\, Au \subset \mathrm{WF}_h\, u.$$

*Moreover*

$$Au = O(h^\infty) \Longrightarrow \mathrm{WF}\, u_h \subset \{\sigma_h(A) = 0\}.$$

The first statement is that PsiDOs are *microlocal*: they don't move WF around. The second (which follows easily from the defintion) is that a family $u$ satisfying an equation must be concentrating in phase space at the *characteristic set* of the equation.

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[8] This result is important in getting intuition for WF, but there is a serious swindle in this statement that I should confess to: in order for it to be true, you have to make an appropriate extension of WF to "fiber infinity." The enemy is, e.g., a distribution like $e^{ix/h^2}$, which is oscillating faster than $e^{i\alpha x/h}$ for any finite $\alpha$. If e.g. $u$ solves an equation like $(h^2\Delta + V - E)u = 0$, this is automatically ok owing to ellipticity of $\Delta$ and you don't have to worry about this extra piece of WF.

2.2. **Defect Measure.** Let $u(x;h)$ be a semiclassical family of distributions. For technical reasons, we will assume throughout this lecture that the family $u(\cdot,h)$ is locally uniformly bounded[9] in $L^2$ as $h \downarrow 0$.

We will start with a non-microlocal notion, measuring concentration in *position space*. For a given $a(x) \in \mathcal{C}_c^\infty(\mathbb{R}^n)$, consider

$$\langle au, u\rangle = \int a(x)|u(x,h)|^2\,dx,$$

as a function of $h \downarrow 0$. (In QM this is the expectation value of the observable $a(x)$ on the quantum wavefunction $u$.) These numbers are bounded (by the locally uniformly $L^2$ hypothesis), but not in general convergent; we can of course extract a sequence of decreasing $h_j \downarrow 0$ so they converge. Let's do so. Indeed, by extracting successive subsequences, we can make

$$\langle a_k u, u\rangle$$

converge for any sequence of $a_k$ that we like. By further extracting a *diagonal subsequence* we may assume that they *all* converge for a specific subsequence $u(x;h_j)$. Let's do this where we have chosen $a_k$ be set of functions that are dense with respect to sup norm in smooth functions supported in every compact set in $\mathbb{R}^n$. Then for any other $f \in \mathcal{C}_c^\infty(\mathbb{R}^n)$, we can easily check that $\langle fu, u\rangle$ converges too, by density!

*Exercise* 10. Check this.

Now given $a \in \mathcal{C}_c^\infty(\mathbb{R}^n)$ let

$$\mu(a) \equiv \lim_{j\to\infty} \langle a(x)u(x;h_j), u(x;h_j)\rangle.$$

This is nonnegative if $a$ is, of course. By Cauchy–Schwarz

$$|\mu(a)| \leq \sup_h \|u(\bullet,h)\|_{L^2(\operatorname{supp} a)} \cdot \sup|a|$$

Thus by Riesz, $\mu$ *is a (positive) Radon measure*! We say $\mu$ is a *semiclassical defect measure* for the family $u$. It is by no means unique in general: recall we built it by extracting nested subsequences to make good things happen. We say that $u$ is a pure sequence if it has only one defect measure.

*Exercise* 11. Find all defect measures associated to the family $h^{-1/2}e^{-x^2/2h}$ in $\mathbb{R}$.

*Exercise* 12. Find all defect measures associated to the family $\phi(x-1/h)$ in $\mathbb{R}$, where $\phi$ is a fixed $L^2$-normalized function.

*Exercise* 13. Show that if $u$ is a pure sequence with defect measure $\mu$ then $x_0 \notin \operatorname{supp}\mu$ iff there is a neighborhood of $x_0$ on which $u = o_{L^2}(1)$ as $h \downarrow 0$. (Contrast this with the notions of WF and essential support, which measure where $u$ lives mod $O(h^\infty)$.)

[9] It suffices to the family to be $h$-tempered—see Dyatlov–Zworski Section E.3.

Now we do the same in phase space! We just replace $a(x)$ with $A = \mathrm{Op}(a(x,\xi)$, the quantization of a symbol $a \in \mathcal{S}(\mathbb{R}^n)$. We say $\mu$, a measure on $T^*\mathbb{R}^n$, is a (semiclassical) *microlocal* defect measure for a family $u$ if along some subsequence,

$$\langle \mathrm{Op}(a)u(\bullet, h_j), u(\bullet, h_j)\rangle \to \int a\, d\mu$$

*Defect measures exist* for any sequence by the same kind of diagonalization and density argument as we used above or the special case of $A = a(x)$.

*Exercise* 14. Show that the only defect measure for the sequence $e^{i\alpha\cdot x/h}$ is Lebesgue measure on the set $\{x \in \mathbb{R}^n,\ \xi = \alpha\}$.

*Exercise* 15. Show that the family of functions on $\mathbb{R}^2$

$$u(x,y;h) = \begin{cases} e^{ix/h}, & \{h^{-1}\} \in [0,1/2), \\ e^{iy/h}, & \{h^{-1}\} \in (1/2,1) \end{cases}$$

(stupidly) has more than one defect measure. (Here $\{\bullet\}$ denotes fractional part.)

*Exercise* 16. Let $u(x,h)$ be the sequence of all solutions to $(h^2\Delta - 1)u = 0$ on the standard 2-torus, hence we are considering a discrete sequence of values of $h$ with $h^{-2} = m^2 + n^2$, $m, n \in \mathbb{Z}$. (I.e., we are studying eigenfunctions of the Laplacian.) What defect measures can you produce along subsequences?

*Exercise* 17. What defect measures does the sequence $e^{ix/h^2}$ have?

**Proposition 8.** *Defect measure is coordinate invariant in $T^*\mathbb{R}^n$.*

**Proposition 9.** *Let $P \in \Psi_h(\mathbb{R}^d)$. If $Pu = o_{L^2}(1)$ and $\mu$ is any defect measure of $u$ then*

$$\operatorname{supp}\mu \subset \{\sigma_h(P) = 0\} \equiv \Sigma.$$

*Proof.* Let $\rho = (x_0, \xi_0) \notin \Sigma$. By use of a *microlocal elliptic parametrix*, if we choose $B = \mathrm{Op}_h(b)$ with $b \geq 0$, $b(\rho) > 0$ and $\operatorname{supp} b \cap \Sigma = \emptyset$, we can *factor* $B = GP + h^\infty R$ for $G, R \in \Psi_h(\mathbb{R}^n)$. (The crucial point is that $b$ is divisible by $\sigma_h(P)$.) Then

$$\langle Bu, u\rangle = \langle GPu, u\rangle + h^\infty\langle Ru, u\rangle = o(1)$$

(since $G$ is uniformly $L^2$-bounded). Hence $\int b\, d\mu = 0$, which yields $\rho \notin \operatorname{supp}\mu$. □

*Exercise* 18. Prove the existence of the factorization used above, e.g. by an iterative construction such as was used in constructing the inverse of an elliptic operator in the "Tools of semiclassical analysis" lectures.

Let's study the sequence $u = b(x)e^{i\phi(x)/h}$, familiar from our previous lecture. For $\operatorname{supp} a \cap \operatorname{supp} b = \emptyset$,

$$\langle au, u\rangle = 0$$

so certainly this shows that[10] $\int a(x)\,d\mu = 0$, hence the support of $\mu$ is within $\operatorname{supp} b$. Note that since $\int \psi(x)\,d\mu = \lim \int \psi |u|^2\,dx = \int \psi |b|^2\,dx \neq 0$ for a bump function $\psi$ of space variables only supported in the interior of $\operatorname{supp} b$, it has a nontrivial defect measure over every point in $\operatorname{supp} b$, and indeed, the same holds upon localizing near any point in $\operatorname{supp} b$, hence there is *some* point in the support of the defect measure over any point in $\operatorname{supp} b$. Now we note

$$(hD_j - \partial_j \phi)u = O_{L^2}(h),$$

since this operator annihilates the oscillating term, while derivatives hitting $b$ are $O(h)$. Hence Proposition 9 shows that for any defect measure $\mu$,

$$\operatorname{supp} \mu \subset \operatorname{graph}(d\phi).$$

Since we knew there was some point in the defect measure over each point, this is it: we've found that the support of the defect measure is $\operatorname{graph}(d\phi) \subset T^*\mathbb{R}^n$.

Let's take stock of this result: remember that $\Lambda = \operatorname{graph}(d\phi)$ was exactly the important submanifold of $T^*\mathbb{R}^n$ that arose in solving the eikonal equation last time! So for our WKB solutions, the locus of concentration in phase space, as measured by the defect measure, is *exactly* this crucial manifold.

Now recall that we could solve for WKB solutions across a hypersurface: once we knew a piece of $\Lambda$, flowing it out along the Hamilton vector field $\mathsf{H}$ gave more of it. This tells us that the support of the defect measures in the special case of WKB solutions are *propagated* along the Hamilton flow. This fact is the tip of a beautiful iceberg.

**Theorem 10.** *Let $P \in \Psi_h(\mathbb{R}^n)$ be a self-adjoint operator, with $Pu = o_{L^2}(h)$ (and $u$ locally uniformly $L^2$). Let $\mu$ be any defect measure for $u$. Then*

$$\operatorname{supp} \mu \subset \{\sigma_h(P) = 0\}$$

*and $\mu$ is invariant under the Hamilton flow of $P$.*

Note that the statement $\operatorname{supp} \mu \subset \{\sigma_h(P) = 0\}$ is just a repeat of what we said before in Proposition 9.

I've stated this pretty generally, so should explain notation. For a general $P$ with symbol $p$, the Hamilton vector field is defined as

$$\mathsf{H}_p \equiv \frac{\partial p}{\partial \xi} \cdot \partial_x - \frac{\partial p}{\partial x} \cdot \partial_\xi.$$

This is in fact invariantly defined on the (symplectic) manifold $T^*\mathbb{R}^n$, if you want to get fancy, by

$$\iota_{\mathsf{H}_p} \omega = -dp$$

where $\omega = d\xi \wedge dx$ is the symplectic form.

*Exercise* 19. (For the geometric sophisticates.) Show these definitions coincide.

[10] Confessing a cheat: $a$ is not actually a Schwartz symbol. It's ok.

*Exercise* 20. (Easy, essentially discussed yesterday:) Check that Hamilton's equations for $p = (1/2)|\xi|^2 + V(x)$ give Newton's law for motion in a potential.

Remember that it's nice to define the *Poisson bracket* of two smooth functions by

$$\{a, b\} = \mathsf{H}_a(b),$$

and an important property of Hamilton vector fields is that this operation is *anticommutative*:

$$\{a, b\} = -\{b, a\}.$$

*Exercise* 21. Check not just that the Poisson bracket is anticommutative, but that it also satisfies the *Jacobi identity*

$$\{\{a, b\}, c\} + \{\{b, c\}, a\} + \{\{c, a\}, b\} = 0,$$

thereby making smooth functions on phase space into a Lie algebra.

The flow along the Hamilton vector field is just the transformation of phase space given by evolving according to Hamilton's equations of motion with Hamiltonian $p$. In other words, it's classical dynamics. The Poisson bracket of $a$ and $b$ is the derivative of the classical observable $b$ under the time-evolution for the system in which we regard $a$ as the Hamiltonian (a.k.a. energy function); the anti-symmetry is, from this point of view, perhaps rather surprising.

What does it mean for $\mu$ to be invariant, as in the statement of the theorem? Let

$$\Phi_t = \exp_{t\mathsf{H}_p}$$

denote the time-$t$ flow. We can evolve a test function $a$ to $\Phi_t^* a \equiv a \circ \Phi_t$ (thus pulling back the function, in geometric terminology). So we can, dually, regard this as pushing forward the measure:

$$(\Phi_t)_*\mu(a) = \mu(\Phi_t^* a) = \int a \circ \Phi_t \, d\mu.$$

(Here we also use the analysts' notation $\mu(f) \equiv \int f \, d\mu$.) Invariance is then the statement that $(\Phi_t)_*\mu = \mu$, i.e., that for any $a$,

$$\int a \circ \Phi_t \, d\mu = \int a \, d\mu. \tag{10}$$

So our punchline is that the main concentration in phase space of $u$ is on a set invariant under the classical dynamics!

What will it take to prove (10)? Since the RHS is exactly the LHS at $t = 0$, it will of course suffice to show the time derivative is zero. What's the derivative? We get exactly

$$\frac{d}{dt} \int a \circ \Phi_t \, d\mu = \int \mathsf{H}_p(a \circ \Phi_t) \, d\mu,$$

hence it will suffice to show that

$$\int \mathsf{H}_p(a)\, d\mu = 0$$

for *all* functions $a$.

Let's now prove this invariance statement; it's surprisingly easy given the tools we now have available. For any $A = \mathrm{Op}(a)$, with $a$ real, let's write the pairing of the commutator of $P$ with $A$ with the function $u$:

$$\frac{i}{h}\langle [P, A]u, u\rangle = \frac{i}{h}\big(\langle Au, Pu\rangle - \langle Pu, A^* u\rangle\big) = o(1)$$

since $P$ is self-adjoint, and since $Pu = o_{L^2}(h)$.

On the other hand, remember the very important relationship between commutators of operators and Poisson brackets of symbols:

$$\frac{i}{h}[P, A] = \mathrm{Op}\{p, a\} + hR = \mathrm{Op}(\mathsf{H}_p(a)) + hR$$

for some remainder $R \in \Psi_h(\mathbb{R}^n)$. So putting together what we know, we find that

$$\langle \mathrm{Op}(\mathsf{H}_p(a))u, u\rangle + h\langle Ru, u\rangle = o(1),$$

hence

$$\langle \mathrm{Op}(\mathsf{H}_p(a))u, u\rangle = o(1).$$

But the LHS is converging to $\mu(\mathsf{H}_p(a))$, hence

$$\mu(\mathsf{H}_p(a)) = 0$$

for all $a$. This completes our proof of invariance of defect measure.

Optional extra: it would be nice to know that defect measures were nonzero in some circumstances. This turns out to correspond to a requirement that mass not escape to infinity in either space or frequency, and is guaranteed if $u$ satisfies an equation where the characteristic set is compact; imagine, e.g., the harmonic oscillator eigenfunctions, given by

$$(h^2\Delta + |x|^2 - E)u = 0.$$

**Proposition 11.** *Let $P = \mathrm{Op}(p) \in \Psi_h(\mathbb{R}^n)$ with $\Sigma = \{p = 0\}$ compact and $p$ bounded below near infinity.*[11] *Suppose $\|u(\bullet, h)\| = 1$ for all $h$ and that*

$$Pu = o(1).$$

*Then every defect measure of $u$ is a probability measure.*

The proof is roughly as follows: pick $a \in \mathcal{C}_c^\infty(T^*\mathbb{R}^n)$ with $a = 1$ on a neighborhood of $\Sigma$. Then we can factor

$$(I - A) = QP + hR$$

[11] Say, elliptic in an appropriate sense; I'm being intentionally vague.

by microlocal elliptic regularity. Thus for each $h$,

$$\begin{aligned}1 &= \langle u, u\rangle \\ &= \langle Au, u\rangle + \langle QPu, u\rangle + h\langle Ru, u\rangle \\ &= \langle Au, u\rangle + o(1),\end{aligned}$$

and the RHS thus approaches $\mu(a)$. Hence $\mu(a) = 1$. But since $\operatorname{supp}\mu \subset \Sigma$ and $a = 1$ on $\Sigma$, this gives

$$\int 1\, d\mu = 1$$

as desired.

A final word on what we haven't said for lack of time: we can also consider propagation of *wavefront set*. It satisfies similar properties to the defect measure: if $Pu = 0$ then the set $\mathrm{WF}_h\, u$ lies in the characteristic set of $P$ and is invariant under the Hamilton flow. The proof of this is a little more involved than the defect measure statement, but similar in flavor.