BULLETIN (New Series) OF THE
AMERICAN MATHEMATICAL SOCIETY
Volume 6, Number 3, May 1982

SINGULARITIES OF SOLUTIONS OF SOME SCHRÖDINGER EQUATIONS ON $\mathbf{R}^n$

BY ALAN WEINSTEIN AND STEVEN ZELDITCH[1]

The Schrödinger equation for the wave function $\psi(t, x_1, x_2, \ldots, x_n)$ for a system of n one-dimensional oscillators is (in suitable units and coordinates)

$$i\hbar \frac{\partial \psi}{\partial t} = H_0 \psi \quad \text{where } H_0 = \sum_{j=1}^{n} \left(\frac{-\hbar^2}{2} \frac{\partial^2}{\partial x_j^2} + \frac{\omega_j}{2} x_j^2 \right).$$

The fundamental solution (or "propagator") $k_0(t, x, y)$ of this equation, with initial condition $k_0(0, x, y) = \Pi_{j=1}^n \delta(x_j - y_j)$, has singularities which can easily be determined by using a well-known explicit formula for k_0 [2, 6] for $t \neq m\pi/\omega_j$ and taking distribution limits as $t \longrightarrow m\pi/\omega_j$.

The result is:

(i) if $l_j = \omega_j t/\pi$ is not an integer for any j, then $k(t, x, y)$ is smooth in x;

(ii) if $l_j \in \mathbf{Z}$ for $j = j_1, \ldots, j_r$ then $k(t, x, y)$ is a smooth δ-function supported on the $(n - r)$-dimensional plane $\{x_{j_s} = (-1)^{l_{j_s}} y_{j_s}\}$.

In quantum mechanics, $k(t, x, y)$ is the (probability) amplitude that a particle *certainly* at y at time 0 has arrived at x at time t. Semi-classically, $k(t, x, y)$ describes a swarm of classical particles with initial positions all at y and with initial momenta uniformly distributed through $\mathbf{R}^n$. The occurrence of singularities in $k(t, x, y)$ coincides with the appearance of an "infinite density" of classical particles at a given point.

In this announcement, we show how this description of singularities can be extended to the case where the Hamiltonian is $H_0 + V$, V being (multiplication by) a potential function on $\mathbf{R}^n$ which is assumed to belong to the symbol class $S^0(\mathbf{R}^n)$; i.e. $|\partial_x^\alpha V| = O(\langle x \rangle^{-|\alpha|})$ for all multi-indices $\alpha \geqslant 0$, where $\langle x \rangle = (1 + |x|^2)^{1/2}$. Semi-classically, the swarm is now additionally influenced by the force $-\text{grad } V(x)$; since this force approaches 0 at ∞, the higher energy particles in the swarm are little influenced by the perturbation, and so they will tend to re-accumulate at the same points as before. It turns out that these points also form the singular locus for the perturbed wave functions, demonstrating the stability of the picture described in (i), (ii) above.

Received by the editors November 25, 1981.

1980 *Mathematics Subject Classification*. Primary 35S10; Secondary 81C05.

[1]Research of first two authors partially supported by NSF grants MCS 77-23579 and MCS 80-12223.

Most of the following theorem was proved in the second author's Ph.D. thesis [9]; part of the results are reproven and slightly sharpened, with their geometric content explicated, in [8].

THEOREM. *Let $\psi_t(x) = \psi(x, t)$ be a tempered distribution solution of the Schrödinger equation*

$$i\hbar \frac{\partial \psi}{\partial t} = \left[\sum_{j=1}^{m} \left(\frac{-\hbar^2}{2} \frac{\partial^2}{\partial x_j^2} + \frac{\omega_j^2}{2} x_j^2 \right) + V(x) \right] \psi$$

with $V \in S^0(\mathbf{R}^n)$. Then

(i) *if $\psi_0 \in E' + S$ (compactly supported plus a Schwartz function), and if t is not an integer multiple of any of the half-periods $\frac{1}{2}T_j = \pi/\omega_j$ then ψ_t is C^∞ (this applies also if all $\omega_j = 0$);*

(ii) *if all frequences ω_j are equal, and $t = l\pi/\omega_j$, $l \in Z$, then* $\mathrm{WF}(\psi_t)$ *is obtained from* $\mathrm{WF}(\psi_0)$ *by multiplying all $2n$ coordinates in $\mathbf{R}^{2n}$ by $(-1)^l$, just as if V were zero. Moreover $\psi_t \in E' + S$ if $\psi_0 \in E' + S$;*

(iii) *if $\omega_j t/\pi = l_j \in Z$ for $j = j_1, \ldots, j_r$, then the singular support of $k(t, \cdot, y)$ is contained in the union of hyperplanes $\{x | x_{j_s} = (-1)^{l_{j_s}} y_{j_s}\}$ (if the ratios ω_j/ω_l are all irrational, the singular support is the same as if V were* 0.)

Most previous work on the Schrödinger equation has dealt with the classical limit (asymptotics as $\hbar \longrightarrow 0$), or has required that the perturbation V be a pseudo-differential operator whose symbol $V(x, \xi)$ belongs to $S^0(\mathbf{R}^{2n})$ **[1, 4, 5, 7]** (these latter can never be multiplication operators). Our results involve the use of a new class of symbols introduced in [9] as amplitudes of operator kernels and adapted in [8] to Weyl symbols. This class consists of functions ("bi-symbols") $a(x, \xi)$ on $\mathbf{R}^{2n}$ for which $\langle x\rangle^k/\langle\xi\rangle^k |D_x^\alpha D_\xi^\beta a|$ and $\langle\xi\rangle^l/\langle x\rangle^l |D_x^\alpha D_\xi^\beta a|$ are bounded whenever $0 \leqslant k \leqslant |\alpha|$, and $0 \leqslant l \leqslant |\beta|$. The corresponding class of pseudo-differential operators is shown to be closed under composition and to permit the solution of evolution equations by series methods. These operators also decrease wavefront sets and preserve smoothness at infinity.

Briefly, the operator equation $i\hbar\, dU/dt = HU$ for the evolution operator $U(t)$ with initial value $U(0) = I$ is solved in the form $U = BU_0$ where U_0 solves the (unperturbed) harmonic oscillator equation $i\hbar\, dU_0/dt = H_0 U_0$. The operator B is then $U_0 A U_0^{-1}$, where A is a solution of

$$i\hbar \frac{dA}{dt} = V(t)A(t) \tag{1}$$

with $V(t) = U_0(t)^{-1} V U_0(t)$. Now the operators $U_0(t)$ belong to the metaplectic representation [5, 7], so the Weyl symbol of $V(t)$ is just the composite of the symbol of V with the time t map of the classical phase flow of the harmonic oscillator system. (More concretely, use the explicit expression for the kernel of U_0 above and a simple change of variables to get

$$U_0^{-1} V U_0 f(x) = \iint dx\, e^{i(x-y)\cdot \xi}\, V([(x+y)/2] \cos t - \xi \sin t) f(x).$$

Then note that in the Weyl calculus, the symbol of this is $V(x \cos t - \xi \sin t)$.)

To solve (1), we rewrite it as the integral equation

$$A(t) = I + \frac{1}{i\hbar} \int_0^t V(s) A(s)\, ds \tag{2}$$

and iterate to get

$$A(t) = I + \sum_{n=1}^{\infty} \left(\frac{1}{i\hbar}\right)^n \int_0^t \cdots \int_0^{s_{n-1}} V(s_1) \cdots V(s_n)\, ds_1 \cdots ds_n.$$

The first term ($n = 1$) is $\int_0^t V(s) ds$, whose Weyl symbol is then

$$\int_0^t V(x \cos s - \xi \sin s) ds.$$

The origin of the bi-symbol calculus lies in the following elementary estimate:
$|\partial_x^\alpha \partial_y^\beta \int_0^t V(x \cos s - \xi \sin s) ds|$

(a) $\leqslant \int_0^t |V^{(\alpha+\beta)}(x \cos s - \xi \sin s)|\, |\cos s|^{|\alpha|} |\sin s|^{|\beta|} ds,$

(b) $\leqslant C_{\alpha\beta} \int_0^t \langle x \cos s - \xi \sin s\rangle^{-|\alpha+\beta|} |\cos s|^{|\alpha|} |\sin s|^{|\beta|} ds,$

(c) $\leqslant C_{\alpha\beta} \sqrt{2} \int_0^t \langle x \cos s\rangle^{-k} \langle \xi \sin s\rangle^{k} |\cos s|^{|\alpha|} |\sin s|^{|\beta|} ds,$

(d) $\leqslant A_{\alpha\beta} \langle x\rangle^{-k} \langle \xi\rangle^{k}$ with $k \leqslant |\alpha|$

(and analogously in ξ). (b) follows (a) by the assumption that $V \in S^0(\mathbf{R}^n)$. (c) follows (b) by Peetre's inequality [3, Lemma 6.12], and the fact that $\langle u\rangle^{-1} \leqslant 1$ for any u. (d) follows from (c) by cancellation of the troublesome coefficients $\cos s$, which then makes the bounds on $\langle x\rangle^{-k} \langle \xi\rangle^{k}$ integrable. Passage from (b) to (c) explains the unusual form of the bi-symbol estimates. Passage from (c) to (d) explains why x-derivatives do not yield a great deal of ξ-decay and vice-versa.

Combining these ideas with integration by parts, one may show that each term in the sum for A is a bi-symbol pseudo-differential operator; it also turns out that the bi-symbols may be summed, so that A is a pseudo-differential operator of this kind as well. This accounts for most of (i) and (ii). For (iii) and part of (i), it is necessary to introduce "nonisotropic symbols" in which the variable pairs are treated separately.

To follow the singularities of $\psi(\cdot, t)$ during the times when they are invisible, we introduce in [8] the notion of the metawave front set MWF(u) of a distribution u. MWF(u) is a subset of

$$A_n = \{(\lambda, \rho) | \lambda \text{ is an affine lagrangian subspace of } \mathbf{R}^{2n} \text{ and } \rho \text{ is a ray in the underlying vector space of } \lambda\}.$$

It is defined by the conditions:

(a) the intersection of MWF(u) with the subset of A_n in which λ is "vertical" is the usual WF(u);

(b) MWF(Lu) $= L$ MWF(u) when L belongs to the inhomogeneous metaplectic group, acting on S' by the metaplectic representation, and on A_n by the action of the inhomogeneous symplectic group on $\mathbf{R}^{2n}$.

Some examples and pitfalls connected with this definition are given in [8].

REFERENCES

1. F. A. Berezin and M. A. Shubin, *Symbols of operators and quantization*, Colloq. Math. Soc. (János Bolyai, ed., 5, *Hilbert Space Operators*, Tihany, Hungary, 1970), North-Holland, Amsterdam, London, 1972.

2. R. P. Feynman and A. R. Hibbs, *Quantum mechanics and path integrals*, McGraw-Hill, New York, 1965.

3. G. B. Folland, *Introduction to partial differential equations*, Princeton Univ. Press, Princeton, N. J., 1976.

4. A. Grossman, G. Loupias and E. M. Stein, *An algebra of pseudo-differential operators and quantum mechanics in phase space*, Ann. Inst. Fourier (Grenoble **18** (1968), 343–368.

5. V. Guillemin and S. Sternberg, *The metaplectic representation, Weyl operators, and spectral theory*, J. Funct. Anal. **42** (1981), 128–225.

6. J. M. Souriau, *Construction explicite de l'indice de Maslov, Applications*, Lecture Notes in Math., vol. 570, Springer-Verlag, Berlin and New York, 1977, pp. 76–96.

7. A. Voros, *Asymptotic ħ-expansions of stationary quantum states*, Ann. Inst. H. Poincaré Sect **26** A (N. S.) **26** (1977), 343–403.

8. A. Weinstein, *A symbol class for some Schrödinger equations on* $\mathbf{R}^n$, Amer. J. Math. (to appear).

9. S. Zelditch, *Reconstruction of singularities for solutions of Schrödinger equations*, Ph.D. Thesis, Univ. of California, Berkeley, 1981.

DEPARTMENT OF MATHEMATICS, UNIVERSITY OF CALIFORNIA, BERKELEY, CALIFORNIA 94720

Current address of Steven Zelditch: DEPARTMENT OF MATHEMATICS, COLUMBIA UNIVERSITY, NEW YORK, NEW YORK 10027