Global Fourier Integral Operators and Semiclassical Asymptotics

by

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Abstract

In this paper we introduce a class of semicalssical Fourier integral operators with global complex phases approximating the fundamental solutions (propagators) for time-dependent Schroedinger equations. Our construction is elementary, it is inspired by the joint work of the first author with Yu. Safarov and D. Vasiliev. We consider several simple but basic examples.

Keywords: Fourier integral operator, global phase, Schroedinger equation, fundamental solution, parametrix, semiclassical asymptotics, Maslov index, magnetic field.

1. Introduction

The notion of Fourier integral operator (FIO) plays an important role in partial differential equations. If pseudo-differential operators can be said to arise from quantization of classical observables, FIO's are due to quantization of classical canonical transformations (Egorov's theorem). More precisely, a transformation of a pseudo-differential operator, P, induced by a change of its symbol under a canonical transformation can be realized (to the leading order) by the conjugation, FPF^{-1}, by an appropriate FIO, F. Furthermore, FIO's give a natural construction of approximate fundamental solutions (parametrices) for hyperbolic problems. These two applications are related. Indeed, on the level of symbols (i.e. classical level) a hyperbolic equation is presented by a Hamiltonian flow. The latter is a family of canonical transformations (labelled by the time variable). Lifting this family to the level of operators yields a desired approximate solution. The derivation indicated

* Supported by the Swedish NSRC under Grant M-AA/MA 9364-320.
** Supported by NSERC under Grant No. NA7901 and Magnusosns fond.

above is valid only for sufficiently small times. In general, the construction of a FIO from a flow breaks down at some moment of time due to existence of focal points. To overcome this problem one either uses a sequence of local FIO's or, more generally, constructs a global FIO. Both procedures are rather labor intensive and subtle (see [H1, H2]).

In this paper we propose a fairly elementary construction giving approximate fundamental solutions (or propagators) to the Schrödinger equation

$$i\alpha\frac{\partial\psi}{\partial t} = H_\alpha\psi \ , \tag{1.1}$$

where α is a semiclassical parameter and H_α is an α-differential operator in $\mathbf{R}^n$ (see, e.g., [D,GS,Hel,M,PP,R]), in terms of semiclassical FIO's. The simplicity of our construction is achieved by using in our FIO's complex phases with quadratic imaginary parts. Our approach is inspired by works [LS] and [LSV], where the global parameterization of homogeneous Langrangian distributions was introduced for construction of fundamental solutions of wave equations. There are difinite connections between our approach and the technique of [BU], [B], [Ral] and also the FBI transform studied in [S] and propagation of coherent states [PU]. An interesting idea for a study of propagation of coherent states was recently suggested in [CD].

Note that though often the natural object in a problem at hand is the Schrödinger propagator, a standard approach is to investigate the wave group, the one that solves the wave equation (see e.g. [H2, SV]). The reason for this is that in the standard pseudo-differential set-up the speed of propagation of singularities for the Schrödinger equation is infinite. However, in the semiclassical framework, which, in fact, is more general, one is typically interested in bounded intervals in energy (= spectral parameter) and the speed with which the singularities (= oscillations, in the semiclassical context) propagate is bounded for bounded energy. Thus localizing the construction of an approximate Schrödinger propagator to a part of the phase space, $T^*\mathbf{R}^n$, in which the momentum (=cotangent variable) is bounded, avoids the problem connected with infinite speed of propagation of singularities on one hand and yields an object convenient for applications, on the other (cf. [IS]).

This paper is organized as follows. In section 2 we introduce our main construction and formulate our main theorem. This theorem is proven in Section 3 modulo an important classical statement of independent interest, whose proof is given in Section 4. We use our construction in Section 5 in order to obtain semiclassical asymptotics of solutions of Schrödinger equation (1.1). In particular, we classify the nature of the phase jumps occuring at caustic sets. In Section 6 we apply our construction to time-dependent Hamiltonians of a "quadratic type". Our approach allows us to obtain a pecise formula for the fundamental solution of the corresponding Schrödinger equation via an oscillatory integral. In the last section we clearify the nature of the phase shift appearing for the motion in a singular magnetic potential concentrated at the origin. Some other applications will be presented elsewhere.

In what follows we will be dealing with (vector) functions on $\mathbf{R}^n$ and on $\mathbf{R}^{2n} = T^*\mathbf{R}^n$. For a function $h(x,\xi)$ from $\mathbf{R}^{2n}$ to $\mathbf{R}$, h_x denotes the n-vector $\left(\frac{\partial h}{\partial x_1}, \dots, \frac{\partial h}{\partial x_n}\right)$ (gradient of h in x) and $h_{x\xi}$ the $(n\times n)$-matrix $\left(\frac{\partial^2 h}{\partial x_i \partial \xi_j}, i = 1,\dots,n, j = 1,\dots,n\right)$. For a vector function $x(y,\eta)$ from $\mathbf{R}^{2n}$ to $\mathbf{R}^n$, x_η stands for the $(n\times n)$ matrix $\left(\frac{\partial x_i}{\partial \eta_j}, i = 1,\dots,n, j = 1,\dots,n\right)$, etc. $\|\cdot\|$ will denote the norm in $L^2(\mathbf{R}^n)$ as well as the norm of operators on this space, $x\cdot y = (x,y)$ will denote the real dot product of vectors in $\mathbf{R}^n$.

2. Main result

In this section we present the main result of this paper. We begin with some basic definitions. Let $h(t,x,\xi)$ be a real, smooth function on $\mathbf{R}^1 \times T^*\mathbf{R}^n$ called a Hamiltonian function. We only assume that there are $m > 0$ and $C_{\mu\nu} > 0$, such that for every $(t,x) \in \mathbf{R}^1 \times \mathbf{R}^n$

$$|\partial_x^\mu \partial_\xi^\nu \; h(t,x,\xi)| < C_{\mu\nu}(1 + |\xi|)^m \; . \tag{2.1}$$

As usual we denote $D_x = -i\frac{\partial}{\partial x}$. Let $H_\alpha(t)$ be the α-pseudodifferential operator with the symbol $h(t,x,\xi)$, i.e.

$$\begin{aligned} H_\alpha(t)f(t,x) &= h(t,x,\alpha D_x)f(t,x) \\ &= (2\pi\alpha)^{-n}\int_{\mathbf{R}^n}\int_{\mathbf{R}^n} h(t,x,\xi)e^{i(x-y)\xi/\alpha}f(y)\,dy\,d\xi, \end{aligned} \tag{2.2}$$

defined first on functions $f\in C_0^\infty(\mathbf{R}^n)$. We assume that $H_\alpha(t)$, for every t, has a self-adjoint extention which we continue denoting by the same symbol $H_\alpha(t)$. Let $U(t,s)$ be the (Schrödinger) propagation for $H_\alpha(t)$, i.e. the family of operators solving the equation

$$-\alpha i\frac{\partial}{\partial t}U(t,s)+H_\alpha(t)U(t,s)=0 \quad \text{and } U(s,s)=I\ , \tag{2.3}$$

where I stands for the identity operator.

Our task is to construct α-FIO's, $U_N(t)$, which approximate $U(t,0)$ within $O(\alpha^{N+1-n})$ for any $N\geq 1$. In what follows (x^t,ξ^t) denote the solutions of the Hamiltonian equations

$$\frac{dx^t}{dt}=\frac{\partial h}{\partial\xi}\quad,\quad \frac{d\xi^t}{dt}=-\frac{\partial h}{\partial x}\quad, \tag{2.4}$$

subject to the initial conditions

$$x^t\big|_{t=0}=y\ ,\ \xi^t\big|_{t=0}=\eta. \tag{2.5}$$

Let g_t be the flow generated by h, i.e. $g_t(y,\eta)=(x^t,\xi^t)$.

Consider the action function S defined as

$$S(t,y,\eta)=\int_0^t\left(h_\xi(s,x^s,\xi^s)\cdot\xi^s-h(s,x^s,\xi^s)\right)ds\ . \tag{2.6}$$

Definition 2.1. Given $T>0$ and $\Omega\subset T^*\mathbf{R}^n$, denote by ϕ the class of functions (phase functions) $\varphi=\varphi(t,x,y,\eta)\in C^\infty([0,T)\times\mathbf{R}^n\times\Omega)$ satisfying the following conditions

(1) $\varphi(t,x^t(y,\eta),y,\eta)=S(t,y,\eta)$,

(2) $\varphi_x(t,x^t(y,\eta),y,\eta)=\xi^t(t,y,\eta)$,

(3) $i^{-1}\varphi_{xx}(t,x,y,\eta)\geq 0$, and is independent of x,

(4) $\det(\varphi_{x\eta}(t,x^t(y,\eta),y,\eta))\neq 0$ for $(t,y,\eta)\in[0,T)\times\Omega$.

Conditions (1)-(3) imply that phase functions $\varphi \in \phi$ are polynomials of the second degree with respect to x

$$\varphi(t, x, y, \eta) = S(t, y, \eta) + (x - x^t) \cdot \xi^t + i(x - x^t) \cdot B(x - x^t)/2 \ , \tag{2.7}$$

where $B = B(y, \eta, t)$ is a non-negative definite $n \times n$ matrix $(= i^{-1}\varphi_{xx}(t, x, y, \eta))$.

Remark 2.2. Instead of the condition (3) we could have considered a more general condition $\Re(i^{-1}\varphi_{xx}(t, x, y, \eta)|_{x=x^t}) \geq 0$. This would lead to a wider class of phase function which is useful for analysis on manifolds. The class which is introduced in Definition 2.1 is sufficient, however, for our purposes. In particular, we can choose $B > 0$ and independent of y, η and t.

The following matrix, appearing in (4), plays an important role in our analysis

$$Z(t, x, y) = \varphi_{x\eta}(t, x, y, \eta)\Big|_{x=x^t(y,\eta)} \ . \tag{2.8}$$

Differentiating condition (2) with respect to η, we obtain the following representation of Z:

$$Z(t, y, \eta) = \xi^t_\eta(y, \eta) - iB(t, y, \eta)x^t_\eta(y, \eta) \ , \tag{2.9}$$

where (recall condition (3))

$$B(t, y, \eta) = i^{-1}\varphi_{xx}(t, x, y, \eta) \ . \tag{2.10}$$

We shall show in Lemma 4.1 below that if $\det B \neq 0$, then Z is a non-degenerated matrix for all $0 \leq t < T$. This implies that condition (4) is fulfilled and therefore the class ϕ is not empty.

At $t = 0$ we obviously have that $Z|_{t=0} = I$. To be able to consider the square root of $\det Z$ we introduce the following agreement.

Agreement 2.3. We choose the branch for the function $\arg\det Z$ which is continuous in t for $0 \leq t < T$, and which yields zero for $t = 0$. This choice allows us to define the value of $(\det Z)^{1/2}$ uniquely for all the values of the parameter t, $0 \leq t < T$.

We consider a bounded subset Ω of the phase-space $T^*\mathbf{R}^n$ and a number $T > 0$ satisfying the following condition:

(H) Hamiltonian equations (2.4)-(2.5) have solutions for every $(y,\eta) \in \Omega$ and for $0 \le t < T$, and the Hamiltonian function h is C^∞ on the set $\bigcup_{0\le t<T} g_t(\Omega)$.

We introduce cut-off functions χ, $\theta \in C_0^\infty(\Omega)$, χ, $\theta \ge 0$ and s.t. $\theta \equiv 1$ on suppχ. With χ we associate the α-pseudodifferential operator $\chi = \chi(x, \alpha D_x)$:

$$(\chi f)(x) = (2\pi\alpha)^{-n} \iint e^{i(x-y)\cdot\eta/2} \chi(y,\eta) f(y) d\eta dy \ . \tag{2.11}$$

Now we are ready to formulate our main result:

Theorem 2.3. *Assume condition (H) to be satisfied. Fix functions χ and θ as described in the preceeding paragraph. For any function $\varphi \in \phi$ and integer $N \ge 0$ there is an operator $U_N(t)$ such that (i) the Schwartz kernel of $U_N(t)$ is of the form*

$$U_N(t,x,y) = (2\pi\alpha)^{-n} \int e^{i\varphi/\alpha} u_N(t,y,\eta,\alpha) d\eta \ , \tag{2.12}$$

where $u_N = \sum_{k=0}^{N} \alpha^k v_{(k)} (\det Z)^{1/2}$ with $v_{(k)}$ smooth functions supported in $[0,T) \times \Omega$ and, in particular,

$$v_0(t,y,\eta) = e^{-i\int_0^t \mathrm{sub}h(s,x^s,\xi^s)ds} \theta(y,\eta) \tag{2.13}$$

with $\mathrm{sub}h = -\frac{1}{2i} Trh_{x\xi}$, the subprincipal symbol of h, and (ii) the operators $U_N(t)$ approximate the propagator $U(t,0)$ on Ω in the sense that for any $T_0 < T$

$$\sup_{0\le t\le T_0} \|(U(t,0) - U_N(t))\chi\| \le C\alpha^{N-2n} \ , \tag{2.14}$$

where $C = C(h,\Omega,T_0)$.

The proof of this theorem is given in the next section with the demonstration of one technical statement, namely that the matrix Z is non-degenerate, carried out in Section 4.

We leave out an important question of how the constant in (2.14) depends h, Ω and T, which requires a rather involved analysis. Notice also that (2.12) gives a family of fundamental solutions depending on a choice of the phase function φ (or the matrix B in (2.7)).

3. Proof of Theorem 2.3.

We begin with deriving some simple equalities needed in the proof.

Lemma 3.1. *For all $(t, y, \eta) \in [0, T) \times \Omega$ the action function S defined in (2.6), satisfies the following identities*

$$S_\eta = x^t_\eta \cdot \xi^t \tag{3.1}$$

and

$$S_y = x^t_y \cdot \xi^t - \eta \ . \tag{3.2}$$

Proof. Both sides of (3.1) are equal to zero when $t = 0$ since $S|_{t=0} = 0$ and $x^t{}_\eta \cdot \xi^t|_{t=0} = y_\eta \cdot \eta = 0$. Using (2.6), we find

$$S_t = h_\xi(t, x^t, \xi^t) \cdot \xi^t - h(t, x^t, \xi^t). \tag{3.3}$$

Thus in view of (2.4)

$$\begin{aligned}\frac{\partial}{\partial t} S_\eta &= \frac{\partial}{\partial \eta}(h_\xi \xi^t - h) \\ &= \dot{x}^t \xi^t_\eta + \dot{x}^t_\eta \xi^t - x^t_\eta h_x - h_\xi \xi^t_\eta \\ &= \dot{x}^t_\eta \xi^t + x^t_\eta \dot{\xi}^t = \frac{d}{dt}(x^t_\eta \xi^t) \ .\end{aligned}$$

This leads to (3.1).

Analogously both sides of (3.2) are equal to zero when $t = 0$. Using now (3.3) and (2.4) we have

$$\begin{aligned}\frac{\partial}{\partial t} S_y &= \frac{\partial}{\partial y}(h_\xi \cdot \xi^t - h) = \dot{x}^t \xi^t_y + \dot{x}^t_y \xi^t - x^t_y h_x - h_\xi \xi^t_y \\ &= \dot{x}^t_y \xi^t + x^t_y \dot{\xi}^t = \frac{d}{dt}(x^t_y \xi^t),\end{aligned}$$

which completes the proof. ■

Now we proceed directly to the proof of Theorem 2.3. The proof is straightforward and standard except for one little twist. Since the integration in η is over bounded sets, all the estimates occuring below are elementary. We shall separate the proof into three parts.

Step 1. Substitution.

We look for a α-FIO $U_N(t)$ given by the integral kernel (2.12) which solves the equation

$$\big(\alpha i \frac{\partial}{\partial t} - H_\alpha(t)\big) U_N(t) = R_N(t) \ , \tag{3.4}$$

where R_N is a α-FI0 with the phase φ and a symbol $\alpha^{N+2} r_N$, where $r_N = O(1)$ and $r_N(t,\cdot,\cdot) \in C_0^\infty(\Omega)$. First we compute the integral kernel of the operator $\big(\alpha i \frac{\partial}{\partial t} - H_\alpha(t)\big)$ $U_N(t)$. Taking into account (2.12), the fact that the phase function φ is a quadratic function with respect to x and applying the standard formula for the action of a pseudodifferential operator on an exponential function (see for example [H2]), we obtain

$$\begin{aligned}
&(\alpha i \frac{\partial}{\partial t} - H_\alpha(t)) U_N(t,x,y) \\
&\quad = (2\pi\alpha)^{-n} \int e^{i\varphi/\alpha} \Big[\alpha i \frac{\partial}{\partial t} u_N - \big(g + O(\alpha^2)\big) u_N\Big] d\eta \ ,
\end{aligned} \tag{3.5}$$

where

$$g = \varphi_t + h(t,x,\varphi_x) + \frac{\alpha}{2}\big((B\partial_\xi, \partial_\xi)h\big)(t,x,\varphi_x) \ .$$

Since φ is a non-degenerated phase function and due to condition (2.1), the r.h.s. of (3.5) can be understood as an oscillatory integral. Using (2.4), we find that

$$\begin{aligned}
\varphi_t &= h_\xi(t,x^t,\xi^t)\cdot\xi^t - h(t,x^t,\xi^t) - \dot{x}^t \xi^t + (x - x^t)\dot{\xi}^t \\
&\quad - i(B(x-x^t), \dot{x}^t) + \frac{i}{2}(x-x^t)\cdot \dot{B}(x-x^t) \\
&= -h(t,x^t,\xi^t) - (x-x^t) h_x(t,x^t,\xi^t) - i(B(x-x^t), h_\xi(t,x^t,\xi^t)) \\
&\quad + \frac{i}{2}(x-x^t)\cdot \dot{B}(x-x^t).
\end{aligned} \tag{3.6}$$

Applying the Taylor formula, we obtain that the third and the forth terms on the right hand side of (3.5) can be written as follows

$$\begin{aligned}
h(t,x,\varphi_x) &= h(t,x,\xi^t + iB(x-x^t)) \\
&= h(t,x^t,\xi^t) + h_x(t,x^t,\xi^t)(x-x^t) + i h_\xi(t,x^t,\xi^t) B(x-x^t) \\
&\quad + \sum_{|\nu|=2} \Big((\partial_x^\nu h)(x-x^t)^\nu + i(\partial_x^{\nu_1}\partial_\xi^{\nu_2} h)(x-x^t)^{\nu_1}(B(x-x^t))^{\nu_2} \\
&\quad - (\partial_\xi^\nu h)(B(x-x^t))^\nu \Big)/\nu! + O(|x-x^t|^3)
\end{aligned} \tag{3.7}$$

and

$$\frac{\alpha}{2}\big((B\partial_\xi,\partial_\xi)h\big)(t,x,\varphi_x)=\frac{\alpha}{2}\big((B\partial_\xi,\partial_\xi)h\big)(t,x^t,\xi^t)+\alpha\,O(|x-x^t|)\ . \tag{3.8}$$

Summing up the expressions (3.6)-(3.8), we find that the terms with α^0 and with $(x-x^t)$ cancel. The rest can be rewritten as

$$g=g_1+\frac{\alpha}{2}\big((B\partial_\xi,\partial_\xi)h\big)(t,x^t,\xi^t)+O(|x-x^t|^3)+\alpha O(|x-x^t|)\ , \tag{3.9}$$

where

$$\begin{aligned}g_1=\sum_{|\nu|=2}\Big[&(\partial_x^\nu h)(x-x^t)^\nu+\sum_{\nu_1+\nu_2=\nu}i(\partial_x^{\nu_1}\partial_\xi^{\nu_2}h)(x-x^t)^{\nu_1}\big(B(x-x^t)\big)^{\nu_2}\\&-(\partial_\xi^\nu h)(B(x-x^t))^\nu\Big]/\nu!+i(x-x^t)\cdot\dot B(x-x^t)\ .\end{aligned} \tag{3.10}$$

Step 2. Integration by parts.

In order to obtain the transport equations we integrate by parts in the integral involving g_1. Notice that

$$\frac{\partial}{\partial\eta}e^{i\varphi/\alpha}=\frac{i}{\alpha}e^{i\varphi/\alpha}\varphi_\eta=\frac{i}{\alpha}e^{i\varphi/\alpha}\big(S_\eta-x_\eta^t\xi^t+\xi_\eta^t(x-x^t)-i(B(x-x^t),x_\eta^t)\big).$$

By Lemma 3.1 we find $S_\eta-x_\eta^t\xi^t=0$. Therefore taking into account (2.9), we obtain

$$(x-x^t)e^{i\varphi/\alpha}=-i\alpha Z^{-1}\frac{\partial}{\partial\eta}e^{i\varphi/\alpha}\ . \tag{3.11}$$

Using this equation and integrating twice by parts in order to convert all powers of $(x-x^t)$ into powers of α, we obtain

$$\begin{aligned}\int e^{i\varphi/\alpha}g_1u_N\,d\eta=&\frac{\alpha}{2i}\int e^{i\varphi/\alpha}\Big\{\mathrm{Tr}\big[Z^{-1}(h_{xx}+iBh_{x\xi}\\&+ih_{x\xi}B-Bh_{\xi\xi}B+i\dot B)x_\eta^t\big]u_N+\sum_{|\beta|\le 2}O(\alpha)\partial^\beta u_N\Big\}d\eta\ .\end{aligned} \tag{3.12}$$

Note that the leading order here is produced when the η-derivative is switched from $e^{i\varphi/\alpha}$ onto the remaining (first) power of $x-x^t$. Differentiating Hamilton equations (2.4) with respect to η, we obtain

$$\dot x_\eta^t=h_{\xi x}x_\eta^t+h_{\xi\xi}\xi_\eta^t\quad,\quad\dot\xi_\eta^t=-h_{xx}x_\eta^t-h_{x\xi}\xi_\eta^t\ .$$

This implies

$$
\begin{aligned}
&(h_{xx} + iBh_{x\xi} + ih_{x\xi}B - Bh_{\xi\xi}B + i\dot{B})x^t_\eta \\
&= (h_{xx}x^t_\eta + h_{x\xi}\xi^t_\eta) + iB(h_{x\xi}x^t_\eta + h_{\xi\xi}\xi^t_\eta) + i\dot{B}x^t_\eta \\
&- h_{x\xi}(\xi^t_\eta - iBx^t_\eta) - iBh_{\xi\xi}(\xi^t_\eta - iBx^t_\eta) \\
&= -\dot{Z} - h_{x\xi}Z - iBh_{\xi\xi}Z \ .
\end{aligned}
\tag{3.13}
$$

Finally, collecting together (3.5), (3.9), (3.12) and (3.13) and using (3.11) and integration by parts in order to convert the powers of $x - x^t$ in the remainder in (3.9) into powers of α, we derive

$$
\Big(\alpha i\frac{\partial}{\partial t} - H_\alpha(t)\Big)U_N(t,x,y) = i(2\pi)^{-n}\alpha^{-n+1}\int e^{i\varphi/\alpha}\Big[\frac{\partial}{\partial t} - \frac{1}{2}\mathrm{Tr}(Z^{-1}\dot{Z} + h_{x\xi}) + O(\alpha)\Big]u_N d\eta \ ,
\tag{3.14}
$$

where $O(\alpha)$ is a differential operator in η with coefficients of order α. Consequently, Eqn (3.4) can be rewritten as

$$
i\alpha\Big[\frac{\partial}{\partial t} - \frac{1}{2}\mathrm{Tr}(Z^{-1}\dot{Z} + h_{x\xi}) + O(\alpha)\Big]u_N = \alpha^{N+2}r_N \ .
\tag{3.15}
$$

Now we write $u_N = \sum\limits_{k=0}^{N}\alpha^k u_{(k)}$ and equate in Eqn (3.15) the terms containing the same power of the parameter α, starting with α and ending with α^{N+2}. As a result we obtain the recurrent system of transport equations. The terms with the multiplier α^{k+1} yield the equation

$$
\frac{\partial}{\partial t}u_{(k)} - \frac{1}{2}\mathrm{Tr}(Z^{-1}\dot{Z} + h_{x\xi}))u_{(k)} = O(1)u_{(k-1)} \ ,
\tag{3.16}
$$

where $k = 0, 1, \ldots, N$, $u_{(-1)} = 0$ and $O(1)$ is a differential operator in η with coefficients of order 1 ($O(1) = -\frac{1}{\alpha}O(\alpha)$, where $O(\alpha)$ is the same as in (3.15)). Setting $r_N = -O(1)u_{(N)}$, we arrive at Eqn (3.4) for $U_N(t)$.

Next, we require that

$$
U_N(0) = \theta(x, \alpha D_x) + O(\alpha^{N+1}) \ ,
\tag{3.17}
$$

where θ is a smooth function supported in Ω and s.t. $\theta \equiv 1$ on suppχ (see the paragraph containing Eqn (2.11)) and $O(\alpha^{N+1})$ stands for a bounded operator whose norm is bounded by $C\alpha^{N+1}$. This leads to initial conditions for Eqn (3.16), to derivation of which we proceed.

Using Eqn (2.7) for the phase φ, we obtain

$$U_N(0,x,y) = (2\pi\alpha)^{-n} \int e^{i(x-y)\cdot\eta/\alpha} e^{-(B(0,y,\eta)(x-y),x-y)/2\alpha} u_N(0,y,\eta)d\eta \ . \tag{3.18}$$

Expanding the function $\exp\left[-(B(0,y,\eta)(x-y),x-y)\right]$ in the Taylor series and integrating by parts, we obtain

$$U_N(0,x,y) = (2\pi\alpha)^{-n} \sum_{\ell=0}^{\infty} \frac{\alpha^\ell}{\ell!} \int e^{i(x-y)\cdot\eta/\alpha} A^\ell u_N d\eta \ , \tag{3.19}$$

where the operator A is defined by

$$(Ag)(\eta) = \sum_{k,\ell=1}^{n} \partial^2_{\eta_k\eta_\ell}(b_{k\ell}(0,y,\eta)g(\eta))$$

with $b_{k\ell}$ being the matrix elements of B. Comparing this with (3.17), using the standard definition of a pseudodifferential operator in terms of its symbol, and writting $u_N = \sum\limits_{k=0}^{N} \alpha^k\ u_{(k)}$, we obtain

$$u_{(0)}(0,y,\eta) = \theta(y,\eta) \tag{3.20}$$

and, for $k = 1,2,\ldots,N$,

$$u_{(k)}(0,y,\eta) = -\sum_{\ell=1}^{k} \frac{1}{\ell!}\ A^\ell u_{(k-\ell)}(0,y,\eta) \ . \tag{3.21}$$

Linear differential equations (3.16) with initial conditions (3.20)-(3.21) can be solved explicitly. In particular,

$$u_{(0)}(t,y,\eta) = (\det Z(t,y,\eta))^{1/2} e^{-i\int_0^t \mathrm{sub}h(s,x^s,\xi^s)ds}\theta(y,\eta) \ , \tag{3.22}$$

where, recall sub$h = -\frac{1}{2i}\mathrm{Tr}h_{x\xi}$, and similarly for $u_{(k)}$, $k \geq 1$. The explicit form of the solutions shows that $u_{(k)}(t,\cdot,\cdot) \in C_0^\infty(\Omega)$ for $k \geq 0$ and $0 \leq t \leq T$.

Remark 3.2. Since every $|x-x^t|^2$ is traded for at least the first power of α, when integrating by parts, Eqn (3.16) involves no more than $2(k-|k|)$ derivatives of the coefficients h_k.

Step 3. Error estimate (2.14).

Since $u_N(t,\cdot,\cdot) \in C_0^\infty(\Omega)$ and Ω is compact, we have that $U_N(t,x,\cdot) \in C_0^\infty(\mathbf{R}^n)$. Writing x as $x - x^t + x^t$ and integrating by parts with a help of (3.11), it is easy to convince oneself that $U_N(t,\cdot,y)$ is in the Schwartz class $\mathcal{S}(\mathbf{R}^n)$. The last two properties can be combined into the formula

$$U_N(t,\cdot,\cdot) \in \mathcal{S}(\mathbf{R}^n, C_0^\infty(\Omega)) \ . \tag{3.23}$$

The definition of r_N (see the paragraph after Eqn (3.16)) and an argument similar to one presented above show that

$$\sup_{0\le t\le T} \|R_N(t)\| \le C(h,\Omega,T)\alpha^{N+1-n} \ . \tag{3.24}$$

Now integrating Eqn (3.4), we obtain

$$U_N(t) - U(t,0)U_N(0) = \frac{1}{i\alpha}\int_0^t U(t,s)R_N(s)ds \ . \tag{3.25}$$

Multiplying this by the operator χ from the right and using Eqn (3.24) and the fact that the norm of $U(t,s)$ is uniformly bounded (in fact, is one), we obtain

$$\|\big(U_N(t) - U(t,0)U_N(0)\big)\chi\| \ \le \ C\alpha^{N-2n} \tag{3.26}$$

with $C = C(h,\Omega,T)$, Finally, due to (3.17) and the fact that $\theta \equiv 1$ on suppχ,

$$\|U_N(0)\chi - \chi\| \le C\alpha^{N-2n} \tag{3.27}$$

and therefore (2.14) follows. ■

4. Z-Matrix

The main result of this section is the following

Lemma 4.1. *If $B > 0$ (see (2.10)), then the matrix-function Z introduced in (2.8) is non-degenerate for all values $(t, y, \eta) \in [0, T) \times \Omega$.*

Proof. First we show that

$$(\xi^t_\eta)^T\, x^t_\eta \;=\; (x^t_\eta)^T\, \xi^t_\eta\ , \tag{4.1}$$

where $(\xi^t_\eta)^T$ is the transpose of the matrix ξ^t_η. Indeed, if $t = 0$, then $x^t_\eta = 0$ and (4.1) is obviously fulfilled. Differentiating the left hand side of (4.1) with respect to t and using (2.4), we find

$$\begin{aligned}
\frac{d}{dt}(\xi^t_\eta)^T x^t_\eta &= (\dot{\xi}^t_\eta)^T x^t_\eta + (\xi^t_\eta)^T \dot{x}^t_\eta \\
&= (-h_{xx}x^t_\eta - h_{x\xi}\xi^t_\eta)^T x^t_\eta + (\xi^t_\eta)^T (h_{\xi\xi}\xi^t_\eta + h_{\xi x}x^t_\eta) \\
&= -(x^t_\eta)^T h_{xx} x^t_\eta + (\xi^t_\eta)^T h_{\xi\xi}\xi^t_\eta\ .
\end{aligned}$$

The second term in (4.1) can be treated analogously

$$\begin{aligned}
\frac{d}{dt}(x^t_\eta)^T \xi^t_\eta &= (\dot{x}^t_\eta)^T\ x^t_\eta + (x^t_\eta)^T \dot{\xi}^t_\eta \\
&= (h_{\xi x}x^t_\eta + h_{\xi\xi}\xi^t_\eta)^T \xi^t_\eta + (x^t_\eta)^T (-h_{x\xi}\xi^t_\eta - h_{xx}x^t_\eta) \\
&= -(x^t_\eta)^T h_{xx} x^t_\eta + (\xi^t_\eta)^T h_{\xi\xi}\xi^t_\eta\ .
\end{aligned}$$

This proves (4.1) for all t, $0 \le t < T$.

Since B is a non-degenerate matrix, it suffices to show that $\operatorname{Ker} \overline{Z}^T B^{-1} Z = \emptyset$. Using (4.1), we obtain

$$\overline{Z}^T B^{-1} Z = (\xi^t_\eta + iB\, x^t_\eta)^T B^{-1} (\xi^t_\eta - iB\, x^t_\eta) = (\xi^t_\eta)^T B^{-1} \xi^t_\eta + (x^t_\eta)^T B x^t_\eta\ . \tag{4.2}$$

Let us assume for a moment that $\overline{Z}^T B^{-1} Z c = 0$ for some vector $c \in \mathbf{C}^n$ and t, $0 < t < T$. Then, since $B > 0$, (4.2) implies that $\xi^t_\eta c = x^t_\eta c = 0$. Using (2.5), we also have that $x^s_\eta|_{s=0} = 0$. Therefore the system of ordinary differential equations

$$\dot{x}^t_\eta c = h_{\xi x} x^t_\eta c + h_{\xi\xi}\xi^t_\eta c\ ,$$

$$\dot{\xi}^t_\eta c = -h_{xx} x^t_\eta c - h_{x\xi}\xi^t_\eta c$$

for $x^t_\eta c$ and $\xi^t_\eta c$, obtained from (2.4), together with the equation $\overline{Z}^t B^{-1} Zc\big|_{t=s} = 0$ (see (4.21)), becomes overdetermined. Since on the other hand the non-trivial solutions x^t and ξ^t do exist, this implies that $c = 0$, which proves the lemma. ■

5. Quasi-classical asymptotics of solutions

In this section we study asymptotic behaviour of solutions of the Schrödinger equation

$$i\alpha \frac{\partial \Psi}{\partial t} = H_\alpha(t)\Psi$$

with an initial condition $\Psi\big|_{t=0} = \Psi_{0\alpha} := \Psi_0((y - y_0)/\alpha)$ for some $y_0 \in \mathbf{R}^n$ and $\Psi_0 \in C_0^\infty(\mathbf{R}^n)$. Let $\rho(x)$ be a cut-off smooth function, such that $\rho \equiv 1$ on $\mathrm{supp}\Psi_{0\alpha}$. We write $\Psi_{0\alpha}$ as $\Psi_{0\alpha}(y) = \Psi_{0\alpha}(y)\rho(y) = (2\pi)^{-n}\rho(y)\int \hat{\Psi}_0(\xi)e^{i(y-y_0)\cdot\xi/\alpha}d\xi$, where $\hat{\Psi}_0(\xi)$ is the Fourier transform of $\Psi_0(x)$. Thus it suffices to consider the initial condition

$$\Psi\big|_{t=0} = \rho(x)e^{ix\cdot\eta_0/\alpha}$$

for a fixed vector $\eta_0 \in \mathbf{R}^n$ $(= T^*_{y_0}\mathbf{R}^n)$. For $\alpha \to 0$, such an initial condition is a fast oscillating function.

To be able to formulate the results of this section we need more notations. Let $A = A_1 + iA_2$ be an $n \times n$ complex, symmetric, non-degenerate matrix with $A_1 \geq 0$ (A_1 and A_2 are real symmetric matrices). We denote by $\det_+ A$ the determinant of A with a particular branch of argument. Namely, the branch of argument of $\det_+ A$ is equal to zero when $A_2 = 0$ and continuously extended with respect to A on the set of matrises A with $\Re A \geq 0$, $\det A \neq 0$ (see [HI, Sect 3.4]). This implies, for example, that if $A_1 = 0$, then

$$\arg\det{}_+ A = \frac{\pi}{2}\mathrm{sgn}A_2, \tag{5.1}$$

where $\mathrm{sgn}A_2$ is the signature of A_2.

Let us assume that for a fixed point $(t, y_0, \eta_0) \in [0, T) \times \Omega$ we have

$$\det(x^t_y(y_0, \eta_0)) \neq 0 \ . \tag{5.2}$$

Then for sufficiently small neigbourhoods $V_{x_0^t}$ and V_{y_0} of $x_0^t = x^t(y_0, \eta_0)$ and y_0, the equation

$$x = x^t(y, \eta_0) \ , \qquad x \in V_{x_0^t} \ , \quad y \in V_{y_0} \ , \tag{5.3}$$

has a unique solution in y which is denoted by $y^* = y^*(t, x, \eta_0)$. Finally, we will assume that the phase φ is given by (2.7) with a constant matrix $B \geq 0$.

Theorem 5.1. *Let the conditions of Theorem 2.3 be satisfied and let U_N be the approximate solution (2.12). Assume also that (5.2) is fulfilled and $y^* = y^*(t, x, \eta_0)$ is the unique solution of the equation (5.3). Then for any smooth function $\rho(y)$, $\mathrm{supp}\rho \subset V_{y_0}$, we have*

$$\begin{aligned} &\int U_N(t, x, y)\rho(y)e^{iy\cdot\eta_0/\alpha}dy \\ &\quad = \rho(y^*)e^{iy^*\cdot\eta_0/\alpha}e^{iS(t,y^*,\eta_0)/\alpha}\ e^{i\mathrm{sub}(t)}e^{i\Delta_{\arg}}|\det x_y^t(t, y^*, \eta_0)|^{-1/2} + O(\alpha) \ , \end{aligned} \tag{5.4}$$

where $\mathrm{sub}(t) = \int_0^t \mathrm{sub}h(s, x^s(y^*, \eta_0), \xi^s(y^*, y_0))ds$ *and*

$$\Delta_{\arg} = \Delta_{\arg}(t, y^*, \eta_0) = \frac{1}{2}\Big(\arg\det Z - \arg\det_+(\Phi/i)\Big)(t, y^*, \eta_0) \ , \tag{5.5}$$

$$\Phi = \Phi(t, y, \eta) = \begin{pmatrix} \varphi_{yy} & \varphi_{\eta y} \\ \varphi_{y\eta} & \varphi_{\eta\eta} \end{pmatrix}_{x = x^t(y,\eta)} . \tag{5.6}$$

Proof. Substituting (2.12) into the l.h.s. of (5.4), we conclude that the latter is equal to

$$(2\pi\alpha)^{-n}\iint e^{i\psi/\alpha}U_N(t, y, \eta, \alpha)\rho(y)d\eta dy \ ,$$

where $\psi(t, x, y, \eta) = \varphi(t, x, y, \eta) + y \cdot \eta_0$. We apply the stationary phase expansion to this integral. To this end we first find stationary points of the phase ψ in η and y. Using (2.7), (3.1) and (2.9), we obtain

$$\begin{aligned} \psi_\eta = \varphi_\eta = S_\eta - (x_\eta^t)^T + (x - x^t)\xi_\eta^t - i(x - x^t)Bx_\eta^t + \frac{i}{2}B_\eta(x - x^t)\cdot(x - x^t) \\ = (x - x^t)Z + O(|x - x^t|^2). \end{aligned} \tag{5.7}$$

Since $\det Z \neq 0$, then in a sufficiently small neigbourhood $V_{x_0^t}$ of x_0^t we have

$$\psi_\eta = 0 \quad \Rightarrow \quad x = x^t(y, \eta) \ . \tag{5.8}$$

Moreover, (3.2) implies

$$\begin{aligned}\varphi_y &= S_y - x^t_y \xi^t + (x - x^t)(\xi^t_y)^T - i(x - x^t)B(x^t_y)^T + \frac{i}{2}B_y(x - x^t)\cdot(x - x^t)\\ &= -\eta + (x - x^t)((\xi^t_y)^T - iB(x^t_y)^T) + O(|x - x^t|^2).\end{aligned} \tag{5.9}$$

Thus

$$\psi_y = \varphi + \eta_0 = 0 \quad \text{and} \quad (5.8) \quad \Rightarrow \quad \eta = \eta_0 .$$

This defines the unique stationaty point $(y, \eta) : y = y^*(t, x, \eta_0)$, $\eta = \eta_0$.

Computing the Hessian of the phase function ψ at this stationary point, we notice that it coinsides with the matrix Φ introduced in (5.6). Let

$$Y(t, y, \eta) = (\xi^t_y(y, \eta))^T - iB(x^t_y(y, \eta))^T \ .$$

Using this notation and expressions (5.7) and (5.9), we compute the entries of the matrix (5.6) at the point (y^*, η_0):

$$\varphi_{yy}(t, x^t, y^*, \eta_0) = -x^t_y Y(t, y^*, \eta_0)\ , \quad \varphi_{\eta y}(t, x^t, y^*, \eta_0) = -x^t_y Z(t, y^*, \eta_0)\ , \tag{5.10}$$

and

$$\varphi_{y\eta}(t, x^t, y^*, \eta_0) = -I - (x^t_\eta)^T Y(t, y^*, \eta_0)\ , \quad \varphi_{\eta\eta}(t, x^t, y^*, \eta_0) = -(x^t_\eta)^T Z(t, y^*, \eta_0)\ . \tag{5.11}$$

Obviously

$$\begin{aligned}\begin{pmatrix} (x^t_\eta)^T(x^t_y)^{-1} & -I \\ -I & 0 \end{pmatrix} \cdot \Phi &= \begin{pmatrix} (x^t_\eta)^T(x^t_y)^{-1} & -I \\ -I & 0 \end{pmatrix} \cdot \begin{pmatrix} -x^t_y Y & -x^t_y Z \\ -I - (x^t_\eta)^T Y & -(x^t_\eta)^T Z \end{pmatrix}\\ &= \begin{pmatrix} I & 0 \\ x^t_y Y & x^t_y Z \end{pmatrix}\ .\end{aligned} \tag{5.12}$$

In particular, this implies

$$|\det\Phi(t, y^*, \eta_0)| = |\big(\det(x^t_y)\det Z\big)(t, y^*, \eta_0)|.$$

Using the stationary phase formula (see for example [H I], Section 7.7), we obtain (5.4). The proof is complete. ■

The next lemma gives an explicit formula for $\mathrm{argdet}_+(\frac{1}{i}\Phi)$.

Lemma 5.2. *Let us assume that both $x^t_y(y,\eta)$ and $x^t_\eta(y,\eta)$ are non-degenerate matrices at $(t,y,\eta)\in[0,T)\times\Omega$. Then the matrix $x^t_y x^t_\eta$ is symmetric and*

$$\operatorname{argdet}_+(\Phi/i)(t,y,\eta) = \operatorname{argdet}_+(i(x^t_\eta)^T Z)(t,y,\eta) - \frac{\pi}{2}\operatorname{sgn}(x^t_y x^t_\eta)(t,y,\eta)\ . \tag{5.13}$$

Proof. Using (4.1), (5.10) and (5.11), we obtain

$$\begin{aligned}
\varphi_{\eta y}|_{x=x^t} &= -x^t_y Z = \varphi^T_{y\eta}|_{x=x^t} = -I - Y^T x^t_\eta\ ,\\
\varphi_{\eta\eta}|_{x=x^t} &= -(x^t_\eta)^T Z = -Z^T x^t_\eta\ , \qquad\qquad .\\
\varphi_{yy}|_{x=x^t} &= x^t_y Y = Y^T (x^t_y)^T
\end{aligned} \tag{5.14}$$

Let

$$J = \begin{pmatrix} 0 & -(x^t_\eta)^T \\ x^t_\eta & (x^t_\eta)^{-1}(x^t_y)^T(x^t_\eta)^T \end{pmatrix}\ .$$

Since the matrix J is real,

$$\operatorname{argdet}_+(\Phi/i) = \operatorname{argdet}_+(J^T\Phi J/i)\ . \tag{5.15}$$

Then using the properties (5.14) we find

$$\begin{aligned}
&J^T\Phi J = \\
&\begin{pmatrix} 0 & (x^t_\eta)^T \\ -x^t_\eta & x^t_\eta x^t_y((x^t_\eta)^{-1})^T \end{pmatrix}
\begin{pmatrix} -x^t_y Y & -I - Y^T x^t_\eta \\ -Z^T(x^t_y)^T & -Z^T x^t_\eta \end{pmatrix}
\begin{pmatrix} 0 & -(x^t_\eta)^T \\ x^t_\eta & (x^t_\eta)^{-1}(x^t_y)^T(x^t_\eta)^T \end{pmatrix}\\
&\qquad = \begin{pmatrix} 0 & (x^t_\eta)^T \\ -x^t_\eta & x^t_\eta x^t_y((x^t_\eta)^{-1})^T \end{pmatrix}
\begin{pmatrix} -x^t_y Z x^t_\eta & -(x^t_\eta)^{-1}(x^t_y)^T(x^t_\eta)^T \\ -(x^t_\eta)^T Z x^t_\eta & 0 \end{pmatrix}.
\end{aligned}$$

Finally we obtain

$$J^T\Phi J = \begin{pmatrix} -(x^t_\eta)^T(x^t_\eta)^T Z x^t_\eta & 0 \\ 0 & (x^t_y)^T(x^t_\eta)^T \end{pmatrix} \tag{5.16}$$

Since the left hand side of (5.15) is a symmetric matrix it follows that the matrix $x^t_y x^t_\eta$ is also symmetric. The equations (5.15) and (5.16) together with (5.1) imply

$$\operatorname{argdet}_+(\Phi/i) = \operatorname{argdet}_+(J^T\Phi J/i) = \operatorname{argdet}_+(i(x^t_\eta)^T(x^t_\eta)^T Z x^t_\eta) + \operatorname{argdet}_+(x^t_y x^t_\eta/i)\ ,$$

which yields (5.13). ∎

Formula (5.5) together with (2.9) shows that if $\det(x^t_y(t, y^*, \eta_0)) \neq 0$, then $\Delta_{\arg}$ is a smooth continuous function of t. However if $\det(x^t_y(t, y^*, \eta_0)|_{t=t_0} = 0$ for some t_0, $0 < t_0 < T$, then the value of $\Delta_{\arg}$ might "jump" as t passes through t_0. Thus the degeneracy of the matrix x^t_y is responsible for the appearence of what we call *configuration* type caustics. The next theorem presents an explicit expression for the jump in $\Delta_{\arg}$.

Theorem 5.3. *Suppose that the conditions of Theorem 5.1 are satisfied,* $\det x^t_y(t_0, y^*, \eta_0) = 0$ *for some* $t_0 \in (0, T)$ *and* $x^t_\eta(t_0, y^*, \eta_0)$ *is a non-degenerate matrix. Then*

$$\begin{aligned} &\lim_{t\to t_0+0} \Delta_{\arg} - \lim_{t\to t_0-0} \Delta_{\arg} \\ &= \frac{\pi}{4}\Big(\operatorname{sgn}(x^t_y x^t_\eta)(t_0 - 0, y^*, \eta_0) - \operatorname{sgn}(x^t_y x^t_\eta)(t_0 + 0, y^*, \eta_0)\Big) \ . \end{aligned} \tag{5.17}$$

Proof. The matrix Z is a non-degenerate, smooth matrix with respect to t. This implies that the value of $\arg\det(i(x^t_\eta)^T Z)$ appearing in the right hand side of (5.12) is a smooth function whenever x^t_η is a non-degenerate matrix. Thus we derive Theorem 5.3 from (5.5) and (5.13). ■

Definition 5.4. Let $\gamma : [0, t] \to T^*\mathbf{R}^n$ be the classical path starting at $(y_0, \eta_0) : \gamma(s) = g_s(y_0, \eta_0)$, $0 \le s \le t < T$, satisfying condition (5.2). Then the number

$$-\frac{1}{2\pi}\int_\gamma d\Delta_{\arg}$$

is called the Maslov index of γ.

Remarks: 5.5. The difference between the number of the positive and the negative eigenvalues of the matrix Φ changes by an even integer. Therefore the difference between the signatures in the right hand side of (5.17) equals $k\pi/2$, where $k = 0, \pm 1, \ldots, \pm n$.

5.6. Function (5.5) was studied in [LSV].

6. Quadratic Hamiltonians

Let $Q(t)$ be a smooth, Hermitian $2n \times 2n$ matrix function and $R(t)$, a smooth real $2n$ vector function. Let $z = (x, \xi) \in \mathbf{R}^{2n}$ and introduce a quadratic Hamiltonian function by the formula

$$h(t,z) = \frac{1}{2} z \cdot Q(t) z + R(t) \cdot z \ . \tag{6.1}$$

In this case Hamiltonian system (2.4) with the initial conditions (2.5) can be rewritten as the following system of linear equations

$$\dot{z} = J\big(Q(t) \cdot z + R(t)\big) \ , \qquad z\big|_{t=0} = z_0 = (y, \eta) \ , \tag{6.2}$$

where $J = \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix}$. Let $M(t)$ be the fundamental matrix of system (6.2), i.e. $M(t)$ solves the initial value problem: $\dot{M}(t) = JQ(t)M(t)$ and $M(0) = \begin{pmatrix} I & 0 \\ 0 & I \end{pmatrix}$. Due to the Liouville-Jacobi formula,

$$\det M(t) = \exp\left(\int_0^t \operatorname{Tr} JQ(s) ds \right) \ ,$$

$M(t)$ is a non-degenerate matrix. The solutions z^t of (6.2) can be represented in terms of $M(t)$ as

$$z^t = M(t) \left(z^0 + \int_0^t M^{-1}(s) R(s) \, ds \right) \ . \tag{6.3}$$

Let $m_{ij}(t)$, $i,j = 1,2$, be the matrix elements of $M(t)$. According to (2.7) and (2.8) we find

$$Z(t,y,\eta) = m_{22}(t) - iB(t,y,\eta) m_{12}(t).$$

If we use a matrix B which is independent of (y,η), then the matrix Z is also independent of (y,η) and the first term of the approximation (2.12) to the fundamental solution of Schrödinger equation (1.1) gives, in fact, the exact formula for this solution.

Theorem 6.1. *Let h be the Hamilton function defined in (6.1) and let $B = B(t)$ from (2.7) be an arbitrary positive definite matrix for $t \geq 0$. Then the Schwartz kernel of the*

Schrödinger equation (1.1) is given by the following oscillatory integral

$$U(t,x,y) = (2\pi\alpha)^{-n}(\det Z(t))^{1/2} \int e^{i\varphi/\alpha} d\eta, \tag{6.4}$$

where the phase function φ is defined in (2.7) and (2.6).

Proof. The proof can be seen from (3.9). Since the Hamiltonian function is quadratic with respect to (x,ξ), we have that $g = g_1$. Moreover, if both B and Z are independent of (y,η), then the terms appearing in the sum in (3.12) are equal to 0. ■

Notice that (6.4) gives us a family of solutions of the Schrödinger equation depending on the choice of an axiliary matrix B. If for example

$$h(x,\xi) = \frac{1}{2}\left(|\xi|^2 + |\omega x|^2\right) \tag{6.5}$$

and ω is a matrix independent of t, then the matrix $M(t)$ in (6.3) can be easiely found to be

$$M(t) = \begin{pmatrix} \cos\omega t & \omega^{-1}\sin\omega t \\ -\omega\sin\omega t & \cos\omega t \end{pmatrix}.$$

If now the matrix B is chosen so that $B = \omega$, then we obtain that Z has a particularly simple form

$$Z(t,y,\eta) = \cos\omega t - i\sin\omega t = e^{-it\omega}$$

and therefore

$$(\det Z)^{1/2} = e^{-it\mathrm{Tr}\omega/2}.$$

Remark: 6.2. Notice that $x^t(y,\eta)$ and $\xi^t(y,\eta)$, defined in (6.3), are linear functions with respect to the initial conditions (y,η). Therefore, the phase function in φ in (6.4) is quadratic and the integral (6.4) can be computed. In particular, if h is defined by (6.5), then we obtain the well-known Mehler formula for the propagator of the harmonic oscillator.

7. Schrödinger operator with magnetic potentials.

Now we consider the motion of a particle in a singular magnetic potential concentrated at the origin and having the total flux ψ_0. Then the corresponding vector potential is

$A(x) = (A_1(x), A_2(x)) = \psi_0(-x_2, x_1)/|x|^2$. The Schrödinger operator for a particle moving in such a magnetic field is

$$H_{0\alpha} = \frac{1}{2}(\alpha D_x - A(x))^2 \ , \tag{7.1}$$

and the corresponding Hamiltonian function is $h_0(x,\xi) = \frac{1}{2}(\xi - A(x))^2$. It is a smooth function on $T^*\mathbf{R}^2$ outside the fiber, $\{(x,\xi) : (x,\xi) = (0,\xi) \ , \xi \in \mathbf{R}^2\}$, over 0. The Hamiltonian equations are

$$\begin{cases} \dot{x}_k^t = \xi_k^t - A_k \ , & x_k^t|_{t=0} = y_k \ , \\ \dot{\xi}_k^t = (\xi^t - A)\cdot(A)_{x_k} \ , & \xi_k^t\big|_{t=0} = \eta_k, \end{cases} \qquad k = 1,2 \ . \tag{7.2}$$

This system obviously reduces to the system of ordinary differential equations of the second order

$$\begin{aligned} \ddot{x}_k^t &= \sum_{j=1}^{2}(\xi_j^t - A_j)\big[(A_j)_{x_k} - (A_k)_{x_j}\big] \\ &= (-1)^{k+1}2\pi(\xi_k^t - A_k(x^t))\delta(x^t) \ , \qquad k = 1,2 \ , \\ & x^t|_{t=0} = y \ , \qquad \dot{x}^t|_{t=0} = \eta - A(y) \ . \end{aligned} \tag{7.3}$$

If we assume that x^t stays away from zero, then the equation (7.3) can be easily solved

$$x^t(y,\eta) = (\eta - A(y))t + y \ , \qquad \xi^t(y,\eta) = \eta + A(x^t) - A(y) \ . \tag{7.4}$$

From (7.4) we see that $x^t(y,\eta) = 0$ for some t if and only if $\eta \wedge y := \eta_1 y_2 - \eta_2 y_1 = -\psi_0$. Therefore we assume that in our construction

$$\Omega \subset \{(y,\eta) : \ \eta \wedge y \neq -\psi_0\} \ .$$

Using (2.6) and (7.4), we obtain the expression for the action function

$$\begin{aligned} S(t,y,\eta) &= \frac{1}{2}|\eta - A(y)|^2 t + \int_0^t (\eta - A(y))\cdot A(x^s)\, ds \\ &= \frac{1}{2}|\eta - A(y)|^2 t - (\eta \wedge y + \psi_0)\int_0^t |x^s|^{-2}\, ds \ . \end{aligned} \tag{7.5}$$

The integral on the right hand side multiplying ψ_0 is a correction term to the free motion due to the magnetic flux through the origin.

Simple calculations show that

$$\xi^t_\eta = \begin{pmatrix} (\xi^t_1)_{\eta_1} & (\xi^t_2)_{\eta_1} \\ (\xi^t_1)_{\eta_2} & (\xi^t_2)_{\eta_2} \end{pmatrix} = \begin{pmatrix} 1 + 2x^t_1 x^t_2 |x^t|^{-4} t\psi_0 & ((x^t_2)^2 - (x^t_1)^2)|x^t|^{-4} t\psi_0 \\ ((x^t_1)^2 - (x^t_2)^2)|x^t|^{-4} t\psi_0 & 1 - 2x^t_1 x^t_2 |x^t|^{-4} t\psi_0 \end{pmatrix}.$$

Therefore the determinant,

$$\det \xi_\eta = 1 - t^2 \psi_0^2 |x^t|^{-4} \ ,$$

degenerates on the "sphere" $|x^t| = \sqrt{t|\psi_0|}$. At these points of degeneracy a non-trivial matrix B is necessary for our constructions of the corresponding fundamental solution.

Now we consider a particle in $\mathbf{R}^2$ moving in the singular magnetic field with the vector potential $A(x)$, given above, and in a quadratic "electric" potential:

$$H_\alpha = \frac{1}{2}(\alpha D_x - A(x))^2 + \frac{1}{2}|x|^2. \tag{7.6}$$

The corresponding Hamiltonian function is

$$h(x,\xi) = \frac{1}{2}(\xi - A(x))^2 + \frac{1}{2}|x|^2 \ . \tag{7.7}$$

The solution of the Hamiltonian equations (2.4)-(2.5) for y and η, s.t. x^t avoids the origin, is

$$x^t = \cos(t)y + \sin(t)(\eta - A(y)) \tag{7.8}$$

and

$$\xi^t = -\sin(t)y + \cos(t)(\eta - A(y)) + A(x^t) \ . \tag{7.9}$$

The action function for this model is equal to

$$S(t,y,\eta) = \int_0^t (h_\xi \dot{\xi}^s - h)\, ds$$

$$= \frac{1}{4}\sin(2t)\big(|\eta - A(y)|^2 - |y|^2\big) + \frac{1}{2}\cos(2t) y \cdot \eta - 2\psi_0(\eta \wedge y + \psi_0) \int_0^t |x^s|^2\, ds.$$

By analogy with the previous example we see that the integral on the right hand side of the last expression can be interpred as a correction term to the motion generated by the harmonic oscillator.

References

[BU] V.M. Babich and V.V. Ulin, Complex space-time ray method and "quasiphotons" (in Russian), *Zap. Nauchn. Sem. Leningrad. Otdel. Mat. Inst. Steklov. (LOMI)*, **117**, (1981), 5-11.

[B] V.S. Buslaev, Semi-classical approach for equations with periodic coefficients, *Soviet Math. Uspehy*, **62** (1987), 77-98.

[CR] M Combescure and D. Robert, Propagation d'équation de Schrödinger et approximation semi-classigue, *C.R. Acad. Sci. Paris.* t. 323, Série I (1996), 871-876.

[D] J. Duistermaat, Fourier integral operators, *N.Y., Courant Inst. Lect. Notes* (1971).

[GS] V. Guillemin and S. Sternberg Geometric asymptotics *Math. Surveys* (1977).

[Hel] B. Helffer, Semiclassical analysis for the Schrödinger operators and applications. *Lecture Notes in Mathematics.* **1336**, Springer-Verlag.

[H1] L. Hörmander, Fourier integral operators I. *Acta Math.*, **127** (1971), 79-183.

[H2] L. Hörmander, The analysis of linear partial differential operators. I–IV, Springer-Verlag, Berlin Heidelberg New York Tokyo (1984).

[HR] B. Helfer and D. Robert, Propriértes asymptotiques du spectre d'opérateurs pseudodifferentieles sur $\mathbf{R}^\mathbf{n}$, *Comm. Partial Diff. Equations*, **7** (1982), 795–882.

[I] V. Ivrii, Semiclassical microlocal analysis and precise spectral asymptotics.

[IS] V. Ivrii and I.M. Sigal, Asymptotics of the ground state energy of large Coulomb systems, *Ann. Math.* **138** (1993), 293–335.

[LS] A. Laptev and Yu. Safarov, Global Parametrization of Lagrangian Manifolds and the Maslov Index, Preprint, Linköping University, (1989).

[LSV] A. Laptev, Yu. Safarov and D. Vassiliev, On global representation of Lagrangian manifolds and solutions of hyperbolic equations, *Comm. Pure Appl. Math.* **XLVII** (1994) 1411–1456.

[M] V. Maslov, The complex WKB method in nonlinear equations, Nauka, Moscow, (1977), 1411-1456.

[PU] T. Paul and A. Uribe, The semiclassical trace formula and propagation of wavw packets, *J. Funct. Anal.* **132**, 1 (1995) 192–249.

[PP] V. Petkov and G. Popov, Semi-classical formula and clastering of eigenvalues for Schrödinger operators, *Preprint, Universitdé Nantes* (1995).

[Ral] J. Ralston, Gaussian beams and the propagation of Singularities, *MAA Studies in Mathematics*, **23** (1982).

[R] D. Robert, *Autour de l'Approximation Semi-Classique,* Birkhäuser, Boston, 1987.

[SV] Yu. Safarov and D. Vassiliev, The asymptotic distribution of eigenvalues of partial differential operators, *Transl. of Math. Monographs, ISSN: 0065-9282* **155** (1996).

[Sh] M. Shubin, *Pseudodifferential Operators,* Springer-Verlag, 1987.

[S] J. Sjöstrand, Singularités analytiques microlocales, *Astérisque* **95**, (1982).