

ON THE FUNDAMENTAL SOLUTION OF A PERTURBED HARMONIC OSCILLATOR

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To Olga Alexandrovna Ladyzhenskaya, with respect and admiration

0. Introduction

In the Schrödinger picture, the change in time of the wave function of a quantum system is governed by the Schrödinger equation

$$\frac{1}{i} \frac{\partial}{\partial t} \psi + H\psi = 0,$$

where H is the Hamiltonian of the system (we choose the units so that $\hbar = 1$). If the operator H does not change in time, then, given $\psi(0) = \psi_0$, we have $\psi(t) = e^{-itH}\psi_0$. The fundamental solution of the time-dependent Schrödinger equation is the distributional kernel of the solution operator e^{-itH} .

For a non-relativistic quantum particle of mass 1 moving in the space of n dimensions in a potential field $V(x)$, the operator H has the form

$$(1) \quad H = -\frac{1}{2}\Delta + V(x),$$

where Δ is the Laplacian in \mathbb{R}^n . We will denote the fundamental solution corresponding to H by $E_H(t, x, y)$. In terms of $E_H(t, x, y)$, the solution of the initial value problem

$$(2a) \quad \frac{1}{i} \frac{\partial}{\partial t} \psi(t, x) - \frac{1}{2}\Delta\psi(t, x) + V(x)\psi(t, x) = 0,$$

$$(2b) \quad \psi(0, x) = \psi_0(x),$$

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is given, formally, by the integral $\psi(t, x) = \int E_H(t, x, y)\psi_0(y) dy$. In its turn, $E_H(t, x, y)$ solves (2) with $\psi_0(x) = \delta(x - y)$.

In this paper we address again the problem of regularity of $E_H(t, x, y)$ in the case of a real, infinitely differentiable potential $V(x)$ that grows at infinity as a power function,

$$(3) \quad |V(x)| = O(|x|^\rho) \quad \text{as } |x| \rightarrow \infty,$$

for some $\rho \geq 0$.

If $V(x)$ and all of its derivatives are bounded, then the only singularity of $E_H(t, x, y)$ is at $t = 0$, and $E_H(t, x, y)$ is C^∞ in $t \in \mathbb{R} \setminus 0$, $x \in \mathbb{R}^n$ and $y \in \mathbb{R}^n$. This was proved by [Zelditch, 1983] (see also [Y. Fujiwara & Osborn, 1983], [Kitada, 1988], [Jensen, 1986]). The same regularity property of $E_H(t, x, y)$ in the case of the potentials with sublinear growth, $\rho < 1$, follows from the recent results of [Craig, Kappeler & Strauss, 1995]. Finally, for the subquadratic ($\rho < 2$) potentials, the regularity of the fundamental solution in $t \in \mathbb{R} \setminus 0$, $x \in \mathbb{R}^n$ and $y \in \mathbb{R}^n$ has been proved independently by [Kapitanski & Rodnianski, 1996] and [Yajima, 1996]. Yajima has also shown that if the potential grows faster than quadratically ($\rho > 2$), then $E_H(t, x, y)$ is quite singular everywhere in t , x and y ; see [Yajima, 1996] for details.

The potentials that grow quadratically compose a special, borderline class. In this paper we will be dealing with the quadratic potentials of the form

$$(4) \quad V(x) = \frac{1}{2}|x|^2 + w(x),$$

where $w(x)$ is a subquadratic perturbation. If $w(x) \equiv 0$, the Hamiltonian becomes $H_0 = -\frac{1}{2}\Delta + \frac{1}{2}|x|^2$, and the corresponding equation (2a) is known as the Schrödinger equation for the quantum harmonic oscillator. The fundamental solution in this case is given by the Mehler formula:

$$(5a) \quad E_{H_0}(t, x, y) = \frac{e^{-in\mu(t)/2}}{|2\pi \sin t|^{n/2}} e^{(i/\sin t)\{\cos t \cdot (|x|^2 + |y|^2)/2 - x \cdot y\}},$$

where $\mu(t) = (2k + 1)\pi/2$ for $\pi k < t < \pi(k + 1)$, k integer, and

$$(5b) \quad E_{H_0}(\pi k, x, y) = e^{-ik\pi/2} \delta((-1)^k x - y).$$

One observes that $E_{H_0}(t, x, y)$ is smooth for non-resonant t , and is singular (a δ -function) for resonant t , $t \in \{k\pi : k \in \mathbb{Z}\}$.

It turns out that such a stratification of regularity is stable under reasonable perturbations of H_0 .

S. Zelditch showed that if the perturbation $w(x)$ is bounded, and all its derivatives are bounded, then $E_H(t, x, y)$ is smooth when $t \notin \{k\pi : k \in \mathbb{Z}\}$,

[Zelditch, 1983, Thm. III]. If $w(x)$ satisfies the more restrictive conditions of being of class $S^0(\mathbb{R}^n)$, i.e.,

$$|\partial_x^\alpha w(x)| = O(|x|^{-|\alpha|}) \quad \text{as } |x| \rightarrow \infty, \quad \forall \alpha \in \mathbb{Z}_+^n,$$

then the singular support of $E_H(k\pi, \cdot, y)$ is just one point, $(-1)^k y$, and $E_H(k\pi, x, y)$ is rapidly decreasing in x away from the singularity [Zelditch, 1983, Thm. II]. The latter result was complemented by A. Weinstein, who showed that the wave front set of $E_H(k\pi, \cdot, y)$ is $(-1)^k$ times the wave front set of $\delta(\cdot - y)$ [A. Weinstein, 1985].

On the other hand, D. Fujiwara studied the structure of $E_H(t, x, y)$ for quadratic potentials $V(x)$ more general than (4). He showed that there is always a small time interval $(0, \tau)$ such that $E_H(t, x, y)$ is smooth when $t \in (0, \tau)$ [D. Fujiwara, 1979, 1980].

Our goal in the present paper is to generalize the results of Zelditch and Fujiwara. For the class of potentials that Fujiwara works with, one cannot expect that the singularities of the fundamental solution will appear only at the moments $t = k\pi$. However, if we assume that $V(x)$ is of the form (4) with $w(x)$ that grows slower than $\text{const} \cdot |x|^2$, then we prove that $E_H(t, x, y)$ develops singularities only at the resonant times $\{k\pi : k \in \mathbb{Z}\}$ and is smooth everywhere else. In fact, we work with two slightly different classes of *subquadratic* perturbations $w(x)$ and use two different techniques, originated in [Kapitanski & Rodnianski, 1996] and [Yajima, 1996], to treat them.

The first technique is based on the estimates for the solutions of the Schrödinger equations in certain Hilbert scales of weighted Sobolev spaces. It relates the decay of the initial data to the smoothening of the solutions at the non-resonant times. The results on the fundamental solution then come as a corollary.

With this technique we are able to treat the real-valued, infinitely differentiable perturbations $w(x)$ that satisfy

$$(6) \quad |\partial_x^\alpha w(x)| \leq c_\alpha \langle x \rangle^{\nu|\alpha|}, \quad \forall \alpha \in \mathbb{Z}_+^n, \quad |\alpha| \geq 1,$$

for some $\nu < 1$, where, as usual, $\langle x \rangle$ stands for $\sqrt{|x|^2 + 1}$.

We use the scale of Hilbert spaces $\{H_s : s \in \mathbb{R}\}$ generated by the powers of the selfadjoint operator $\Lambda = (-\Delta + |x|^2 + 1)^{1/2}$ in $H_0 = L^2(\mathbb{R}^n)$. By definition, H_s , for positive s , is the domain of Λ^s equipped with the inner product $(f, g)_s = (\Lambda^s f, \Lambda^s g)$, and H_s is the dual space to H_{-s} when s is negative.

THEOREM I. *Assume that w satisfies (6) with $0 \leq \nu < 1$. Let $\psi^0 \in H_s$, for some s , and, in addition, $\langle x \rangle^l \psi^0 \in H_{s-l\nu}$ for $l = 1, \dots, m$, some integer $m \geq 1$.*

Then for any $t > 0$ the solution ψ of the initial value problem

$$(7a) \quad \frac{1}{i} \frac{\partial}{\partial t} \psi(t, x) - \frac{1}{2} \Delta \psi(t, x) + \frac{1}{2} |x|^2 \psi(t, x) + w(x) \psi(t, x) = 0, \quad t > 0, \quad x \in \mathbb{R}^n,$$

$$(7b) \quad \psi(0, x) = \psi^0(x),$$

has the following regularity properties:

$$(8a) \quad \left(\frac{\sin t}{\langle x \rangle^{1-\nu}} \right)^l \psi(t, \cdot) \in H_{s+l(1-\nu)}, \quad l = 0, 1, \dots, m,$$

and the $H_{s+l(1-\nu)}$ -valued function $(\sin t / \langle x \rangle^{1-\nu})^l \psi(t, \cdot)$ is continuous for $t > 0$. Moreover, given $T > 0$, there exists a constant $c = c(T, m, V) > 0$ such that the following estimate holds:

$$(8b) \quad \left\| \left(\frac{\sin t}{\langle x \rangle^{1-\nu}} \right)^m e^{-itH} \psi^0 \right\|_{H_{s+m(1-\nu)}} \leq c \sum_{l=0}^m \|\langle x \rangle^l \psi^0\|_{H_{s-l\nu}}, \quad \forall t, \quad 0 < t \leq T.$$

This theorem implies immediately the following result.

COROLLARY II. *If $w(x)$ satisfies (6) then the fundamental solution $E_H(t, x, y)$ is C^∞ for $t \notin \pi\mathbb{Z}$. In addition, for any integer $m \geq 0$, and any $\varepsilon > 0$, the functions*

$$\left(\frac{\sin t}{\langle \cdot \rangle^{1-\nu}} \right)^m E_H(t, \cdot, y) \quad \text{and} \quad \left(\frac{\sin t}{\langle \cdot \rangle^{1-\nu}} \right)^m E_H(t, x, \cdot)$$

are continuous functions of t with values in $H_{-n/2-\varepsilon+m(1-\nu)}$.

The second technique is based on Fujiwara's construction of the fundamental solution for small time intervals. Here we need the following assumptions on $w(x)$: $w(\cdot)$ is real-valued, infinitely differentiable, and

$$(9) \quad |\partial_x^\alpha w(x)| = o(1) \quad \text{as } |x| \rightarrow \infty, \quad \forall \alpha \in \mathbb{Z}_+^n, \quad |\alpha| \geq 2.$$

THEOREM III. *Suppose $w(x)$ satisfies (9). Then the fundamental solution $E_H(t, x, y)$ is a C^∞ -function in every slab $\Pi_{k,\varepsilon} = \{(t, x, y) : k\pi + \varepsilon < t < (k+1)\pi - \varepsilon, x, y \in \mathbb{R}^n\}$, $k \in \mathbb{Z}$, $\varepsilon \in (0, \pi/2)$. Moreover, in every layer $\Pi_{k,0}$, the fundamental solution can be written in the form*

$$(10) \quad E_H(t, x, y) = a(t, x, y) e^{i\phi(t, x, y)},$$

where the functions $a(t, x, y)$ and $\phi(t, x, y)$ are infinitely differentiable in $\Pi_{k,0}$, while in the narrower slabs $\Pi_{k,\varepsilon}$, $\varepsilon > 0$, they have the following additional properties:

$$(11a) \quad \sup_{(t,x,y) \in \Pi_{k,\varepsilon}} |\partial_t^l \partial_x^\alpha \partial_y^\beta a(t, x, y)| \leq c_{l,\alpha,\beta}(\varepsilon), \quad \forall l = 0, 1, 2, \dots, \forall \alpha, \beta \in \mathbb{Z}_+^n,$$

$$(11b) \quad \sup_{(t,x,y) \in \Pi_{k,\varepsilon}} |\partial_t^l \partial_x^\alpha \partial_y^\beta \phi(t, x, y)| \leq c_{l,\alpha,\beta}(\varepsilon),$$

$$\forall l = 0, 1, 2, \dots, \forall \alpha, \beta \in \mathbb{Z}_+^n, |\alpha + \beta| \geq 2,$$

for some positive constants $c_{l,\alpha,\beta}(\varepsilon) < \infty$.

In addition, there exists $\varrho = \varrho(\varepsilon) > 0$ such that whenever $|x|^2 + |y|^2 \geq \varrho^2$, the phase function $\phi(t, x, y)$ is the classical action

$$(12) \quad S(t, x, y) = \int_0^t \left(\frac{1}{2} \left| \frac{dx(s)}{ds} \right|^2 - \frac{1}{2} |x(s)|^2 - w(x(s)) \right) ds,$$

where $x(s)$ is the unique classical trajectory connecting $y = x(0)$ with $x = x(t)$. More precisely, if $|x|^2 + |y|^2 \geq \varrho^2$, then, first, there exists a unique solution $x(s)$ of the Newton equation

$$\frac{d^2}{ds^2} x(s) = -x(s) - \frac{\partial w}{\partial x}(x(s)),$$

such that $y = x(0)$ and $x = x(t)$; second, $S(t, x, y)$ is well defined and satisfies (11b); and finally, the phase function in (10) can be chosen so that $\phi(t, x, y) = S(t, x, y)$.

REMARK. The class of potentials satisfying (6) nearly includes all potentials of class (9). But neither of them includes the other. Instructive examples are the following. The potential

$$(13a) \quad w(x) = |x|^2 / \ln \langle x \rangle$$

obeys the conditions (9) but not (6).

The potential

$$(13b) \quad w(x) = \langle x \rangle^{r_1} \sin \langle x \rangle^{r_2},$$

with $r_1, r_2 > 0$ and $r_1 + r_2 < 2$, obeys (6) with any ν such that $r_1 + r_2 - 1 \leq \nu < 1$, but does not obey (9).

REMARK. Since E_H is smooth inside any slab $\Pi_{k,\varepsilon}$, we can always write $E_H(t, x, y)$ in the form (10) with smooth (inside $\Pi_{k,\varepsilon}$) amplitude a and phase ϕ . Note, however, that Corollary II does not give the boundedness of the sort that Theorem III does (see (11)).

Once we know that the fundamental solution $E_H(t, x, y)$ is singular only at the resonant times, the question arises about the structure of the singularities of

$E_H(k\pi, x, y)$. At the moment we do not have in any way complete answers, but a partial result that we have is of interest.

THEOREM IV. *Assume that w is of class \mathcal{S}^ν for some $\nu < 1$, i.e.,*

$$(14) \quad |\partial^\alpha w(x)| \leq c_\alpha \langle x \rangle^{\nu-|\alpha|}, \quad \forall \alpha \in \mathbb{Z}_+^n.$$

Then the singular support of $E_H(k\pi, \cdot, y)$ is $\{(-1)^k y\}$.

REMARK. Thus, the sublinear perturbations do not affect the location of the singularities of the fundamental solution. It is likely that the wave front set is not affected either. Note, however, that for linear $w(x) = c \cdot x$ we have

$$(5a') \quad E_H(t, x, y) = \frac{e^{-in\mu(t)/2}}{|2\pi \sin t|^{n/2}} e^{i|c|^2 t/2} e^{i(\sin t)\{\cos t \cdot (|x+c|^2 + |y+c|^2)/2 - (x+c) \cdot (y+c)\}},$$

and the singularity of $E_H((2m+1)\pi, \cdot, y)$ is now located at $x = -y - 2c$ and not at $x = -y$ as it was in the case $w = 0$.

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1. Estimates in weighted Sobolev spaces

Consider the initial value problem

$$(1.1a) \quad \begin{aligned} \frac{1}{i} \frac{\partial}{\partial t} \psi(t, x) - \frac{1}{2} \Delta \psi(t, x) \\ + \frac{1}{2} |x|^2 \psi(t, x) + w(x) \psi(t, x) = 0, \quad t > 0, \quad x \in \mathbb{R}^n, \end{aligned}$$

$$(1.1b) \quad \psi(0, x) = \psi^0(x).$$

In this section we assume that $w(x)$ is real, infinitely differentiable, and, for some $\nu < 1$, satisfies the conditions

$$(1.2) \quad |\partial_x^\alpha w(x)| \leq c_\alpha \langle x \rangle^{\nu-|\alpha|}, \quad \forall \alpha \in \mathbb{Z}_+^n, \quad |\alpha| \geq 1.$$

We study (1.1) in the scale of Hilbert spaces H_s , $s \in \mathbb{R}$, defined in the introduction. Note that Λ^r is an isometry between H_s and H_{s-r} for any $r \in \mathbb{R}$ and any $s \in \mathbb{R}$. In particular, the following norms are equivalent:

$$(1.3) \quad \|\nabla f\|_{(s)}^2 + \|\langle x \rangle f\|_{(s)}^2 \approx \|f\|_{(s+1)}^2,$$

where $\|\cdot\|_{(s)}$ is the norm in H_s .

A linear operator $A : \bigcup_s H_s \rightarrow \bigcup_s H_s$ is said to be of *order* $\leq r$ if A maps continuously H_s into H_{s-r} for every $s \in \mathbb{R}$. Of course, Λ^r is of order $\leq r$. It is not hard to show that the operator of multiplication by $\langle x \rangle^k$, $k > 0$, is of order $\leq k$, while $\langle x \rangle^k$ with negative k is of order ≤ 0 . A little bit harder is the fact that (multiplication by) $w(x)$ is of order $\leq 1 + \nu$, and the derivatives $\partial_x^\alpha w(x)$ are of order $\leq \nu|\alpha|$ [Kapitanski & Rodnianski, 1996].

Along with (1.1) we consider a more general inhomogeneous problem

$$(1.4) \quad \begin{aligned} \frac{1}{i} \frac{\partial}{\partial t} u(t, x) - \frac{1}{2} \Delta u(t, x) + \frac{1}{2} |x|^2 u(t, x) + w(x) u(t, x) &= h(t, x), \\ u(0, x) &= u_0(x). \end{aligned}$$

The general approach developed in [Kapitanski, 1990], when applied to (1.4), gives the following existence and uniqueness results.

LEMMA 1.1. *For any real r , for any $u_0 \in H_r$ and for any $h(\cdot, \cdot) \in L^1_{\text{loc}}(\mathbb{R} \rightarrow H_r)$, there exists a unique solution $u(t, x)$ of (1.4) such that the corresponding mapping $u : \mathbb{R} \ni t \mapsto u(t, \cdot) \in H_r$ is (strongly) continuous. Moreover, for every $T > 0$, there exists a constant $\tilde{c}_T > 0$ such that the following energy estimate holds:*

$$(1.5) \quad \|u(t, \cdot)\|_{(r)} \leq \tilde{c}_T \left\{ \|u_0\|_{(r)} + \int_0^t \|h(\tau, \cdot)\|_{(r)} d\tau \right\}, \quad 0 \leq t \leq T.$$

This follows from Lemma 2.1 of [Kapitanski, 1990]. The only thing one has to check is that the commutator $[\Lambda^{2k}, w]$ is a continuous mapping from H_k into H_{-k} , for every real k (see [Kapitanski, 1990], Lemma 2.1). But this is true because of (1.2).

We now turn to the proof of Theorem I. The scheme of the proof will be essentially the same as in [Kapitanski & Rodnianski, 1996]. To make the exposition more transparent, we take here $n = 1$. The necessary changes in the case $n > 1$ are outlined in Remark below.

PROOF OF THEOREM I. Our assumptions on the initial wave-function are the following: for some $s \in \mathbb{R}$ and some integer $m \geq 1$,

$$(1.6) \quad \langle x \rangle^l \psi^0 \in H_{s-l\nu}, \quad l = 0, 1, \dots, m.$$

By Lemma 1.1, problem (1.1) has a unique solution $\psi \in C_{\text{loc}}(\mathbb{R} \rightarrow H_s)$, and, for any $T > 0$,

$$(1.7) \quad \sup_{0 \leq t \leq T} \|\psi(t, \cdot)\|_{(s)} \leq \tilde{c}_T \|\psi^0\|_{(s)}.$$

Define an operator

$$(1.8) \quad \mathcal{Y}_t = \cos t \cdot x + i \sin t \cdot \partial_x.$$

Set

$$\mathcal{L} = \frac{1}{i} \frac{\partial}{\partial t} - \frac{1}{2} \Delta + \frac{1}{2} |x|^2 + w(x).$$

It is easy to check that the commutators of \mathcal{L} with the powers of \mathcal{Y}_t can be written in the form

$$(1.9) \quad [\mathcal{L}, \mathcal{Y}_t^N] = - \sum_{k=1}^N \binom{N}{k} ((i \sin t \cdot \partial_x)^k w(x)) \cdot \mathcal{Y}_t^{N-k}.$$

The function $\psi_1 = \mathcal{Y}_t \psi$ is the solution of the following inhomogeneous problem:

$$(1.10) \quad \mathcal{L} \psi_1 = -i \sin t \cdot \partial_x w(x) \cdot \psi, \quad \psi_1(0, x) = x \psi^0(x).$$

In view of our assumption (1.6), we have $\psi_1(0, \cdot) \in H_{s-\nu}$. The operator (of multiplication by) $\partial_x w(x)$ is of order $\leq \nu$. When it acts on $\psi(t, \cdot) \in H_s$, the result lies in $H_{s-\nu}$. Applying Lemma 1.1 to (1.10), we see that $\psi_1 \in C_{\text{loc}}(\mathbb{R} \rightarrow H_{s-\nu})$, and, for any $T > 0$,

$$(1.11) \quad \sup_{0 \leq t \leq T} \|\psi_1(t, \cdot)\|_{(s-\nu)} \leq c_T \{\|x \psi^0\|_{(s-\nu)} + \|\psi^0\|_{(s)}\}.$$

Here and further on, c_T and c stand for constants that do not depend on ψ^0 , but may change from estimate to estimate.

The estimate (1.11) implies that $\langle x \rangle^{-(1-\nu)} (\sin t) \psi \in H_{s+(1-\nu)}$. To see this, we need the following identity:

$$(1.12) \quad \partial_x \left(\frac{(i \sin t)^{k+1} \phi}{\langle x \rangle^{(k+1)(1-\nu)}} \right) = \frac{1}{\langle x \rangle^{1-\nu}} \cdot \frac{(i \sin t)^k \mathcal{Y}_t \phi}{\langle x \rangle^{k(1-\nu)}} - \cos t \cdot \frac{x}{\langle x \rangle^{1-\nu}} \cdot \frac{(i \sin t)^k \phi}{\langle x \rangle^{k(1-\nu)}} \\ - \frac{(k+1)(1-\nu) i \sin t \cdot x}{\langle x \rangle^{3-\nu}} \cdot \frac{(i \sin t)^k \phi}{\langle x \rangle^{k(1-\nu)}}$$

where k is an arbitrary non-negative constant, and ϕ is an arbitrary temperate distribution, say. If $\phi = \psi$, and $k = 0$, then the $H_{s-\nu}$ -norm of the right side of (1.12) is bounded by

$$c(\|\mathcal{Y}_t \psi(t, \cdot)\|_{(s-\nu)} + \|\langle x \rangle^\nu \psi(t, \cdot)\|_{(s-\nu)} + \|\langle x \rangle^{-2+\nu} \psi(t, \cdot)\|_{(s-\nu)}) \\ \leq c(\|\psi_1(t, \cdot)\|_{(s-\nu)} + \|\psi(t, \cdot)\|_{(s)}) \leq c_T(\|\langle x \rangle \psi^0\|_{(s-\nu)} + \|\psi^0\|_{(s)}).$$

Hence,

$$(1.13a) \quad \sup_{0 \leq t \leq T} \left\| \partial_x \left(\frac{\sin t \cdot \psi(t, \cdot)}{\langle x \rangle^{1-\nu}} \right) \right\|_{(s-\nu)} \leq c_T(\|\langle x \rangle \psi^0\|_{(s-\nu)} + \|\psi^0\|_{(s)}).$$

On the other hand,

$$(1.13b) \quad \left\| \langle x \rangle \left(\frac{\sin t \cdot \psi(t, \cdot)}{\langle x \rangle^{1-\nu}} \right) \right\|_{(s-\nu)} \leq c \|\psi(t, \cdot)\|_{(s)} \leq c_T \|\psi^0\|_{(s)}.$$

From (1.13), taking into account (1.3), we obtain the estimate

$$(1.14) \quad \sup_{0 \leq t \leq T} \left\| \frac{\sin t \cdot \psi(t, \cdot)}{\langle x \rangle^{1-\nu}} \right\|_{(s+1-\nu)} \leq c_T (\|\langle x \rangle \psi^0\|_{(s-\nu)} + \|\psi^0\|_{(s)}),$$

which proves our theorem in the case $m = 1$. If $m = 2$, we proceed as follows.

Define $\psi_2 = \mathcal{Y}_t \psi_1 = \mathcal{Y}_t^2 \psi$. Since ψ is the solution of (1.1), ψ_2 is the solution of the problem (we use (1.9) here)

$$(1.15) \quad \mathcal{L}\psi_2 = -i \sin t \cdot \partial_x w(x) \cdot \psi_1 + \sin^2 t \cdot \partial_x^2 w(x) \cdot \psi, \quad \psi_2(0, x) = x^2 \psi^0(x).$$

By assumption (1.6), $\psi_2(0, \cdot) \in H_{s-2\nu}$. The right hand side of the differential equation is a continuous function of t with values in $H_{s-2\nu}$, and its $H_{s-2\nu}$ -norm is bounded by $c_T (\|\langle x \rangle \psi^0\|_{(s-\nu)} + \|\psi^0\|_{(s)})$ on the interval $[0, T]$. This follows from (1.2), (1.7) and (1.11). Lemma 1.1 then implies that $\psi_2 \in C_{\text{loc}}(\mathbb{R} \rightarrow H_{s-2\nu})$ and

$$(1.16) \quad \sup_{0 \leq t \leq T} \|\psi_2(t, \cdot)\|_{(s-2\nu)} \leq c_T \{ \|\langle x \rangle^2 \psi^0\|_{(s-2\nu)} + \|\langle x \rangle \psi^0\|_{(s-\nu)} + \|\psi^0\|_{(s)} \}.$$

In the same fashion as we obtained (1.14), we use the identity (1.12) with $\phi = \psi_1$ and $k = 0$ to show that

$$(1.17) \quad \sup_{0 \leq t \leq T} \left\| \frac{\sin t \cdot \psi_1(t, \cdot)}{\langle x \rangle^{1-\nu}} \right\|_{(s+1-2\nu)} \leq c_T (\|\langle x \rangle^2 \psi^0\|_{(s-2\nu)} + \|\langle x \rangle \psi^0\|_{(s-\nu)} + \|\psi^0\|_{(s)}).$$

The identity (1.12), with $\phi = \psi$ and $k = 1$, reads

$$(1.18) \quad \partial_x \left(\frac{(i \sin t)^2 \psi}{\langle x \rangle^{2(1-\nu)}} \right) = \frac{1}{\langle x \rangle^{1-\nu}} \cdot \frac{(i \sin t) \psi_1}{\langle x \rangle^{1-\nu}} - \cos t \cdot \frac{x}{\langle x \rangle^{1-\nu}} \cdot \frac{(i \sin t) \psi}{\langle x \rangle^{1-\nu}} - \frac{2(1-\nu) i \sin t \cdot x}{\langle x \rangle^{3-\nu}} \cdot \frac{(i \sin t) \psi}{\langle x \rangle^{1-\nu}}.$$

The right side of this equality is in $H_{s+1-2\nu}$, with the norm bounded by

$$c \left(\left\| \frac{\sin t \cdot \psi_1(t, \cdot)}{\langle x \rangle^{1-\nu}} \right\|_{(s+1-2\nu)} + \left\| \frac{\sin t \cdot \psi(t, \cdot)}{\langle x \rangle^{1-\nu}} \right\|_{(s+1-\nu)} \right).$$

Therefore, the estimates (1.14) and (1.17) yield

$$(1.19a) \quad \sup_{0 \leq t \leq T} \left\| \partial_x \left(\frac{(i \sin t)^2 \psi}{\langle x \rangle^{2(1-\nu)}} \right) \right\|_{(s+1-2\nu)} \leq c_T (\|\langle x \rangle^2 \psi^0\|_{(s-2\nu)} + \|\langle x \rangle \psi^0\|_{(s-\nu)} + \|\psi^0\|_{(s)}).$$

At the same time,

$$(1.19b) \quad \left\| \langle x \rangle \left(\frac{(i \sin t)^2 \psi}{\langle x \rangle^{2(1-\nu)}} \right) \right\|_{(s+1-2\nu)} = \left\| \langle x \rangle^\nu \left(\frac{(i \sin t)^2 \psi}{\langle x \rangle^{1-\nu}} \right) \right\|_{(s+1-2\nu)} \\ \leq c \left\| \frac{\sin t \cdot \psi}{\langle x \rangle^{1-\nu}} \right\|_{(s+1-\nu)} \\ \leq c_T (\|\langle x \rangle \psi^0\|_{(s-\nu)} + \|\psi^0\|_{(s)}).$$

In view of (1.3), the estimates (1.19) lead to the estimate

$$(1.20) \quad \sup_{0 \leq t \leq T} \left\| \frac{(i \sin t)^2 \psi(t, \cdot)}{\langle x \rangle^{2(1-\nu)}} \right\|_{(s+2(1-\nu))} \\ \leq c_T (\|\langle x \rangle^2 \psi^0\|_{(s-2\nu)} + \|\langle x \rangle \psi^0\|_{(s-\nu)} + \|\psi^0\|_{(s)}),$$

which proves Theorem I in the case $m = 2$. If $m > 2$, then one has to proceed in the same fashion, improving the regularity of ψ step by step.

2. On the singular supports of the solutions

In this section we prove a theorem that relates the location and strength of the point singularities of the wave function at the resonant times $t = k\pi$, $k \neq 0$, to the location and strength of the singularity at $t = 0$. As in Section 1, we use the scale of weighted Sobolev spaces H_s , the energy estimates, and commutators.

Consider the problem

$$(2.1) \quad \mathcal{L}\psi = 0, \quad \psi(0) = \psi^0,$$

where $\mathcal{L} = \frac{1}{i} \frac{\partial}{\partial t} - \frac{1}{2} \Delta + \frac{1}{2} |x|^2 + w(x)$. In this section we impose stronger restrictions on $w(x)$. Namely, we assume that $w(x)$ satisfies the assumption of Theorem V:

$$(2.2) \quad |\partial^\alpha w(x)| \leq c_\alpha \langle x \rangle^{\nu-|\alpha|}, \quad \forall \alpha \in \mathbb{Z}_+^n, \quad \text{for some } \nu < 1.$$

To state our main result, we first introduce two sets of operators, which act in the scale H_s , and which depend on two parameters: the time, t , and the point $y = (y^1, \dots, y^n) \in \mathbb{R}^n$; the latter may be viewed as the location of the singularity of ψ^0 . The operators in question are

$$(2.3a) \quad \mathcal{K}_t^j = \cos t \cdot x^j + i \sin t \cdot \frac{\partial}{\partial x^j} - y^j, \quad j = 1, \dots, n,$$

$$(2.3b) \quad \mathcal{R}_t^k = -\sin t \cdot x^k + i \cos t \cdot \frac{\partial}{\partial x^k} - y^k, \quad k = 1, \dots, n.$$

We use these operators to state the hypotheses about the initial data and in the proof later on, as well.

We assume that $\psi^0 \in H_s$ for some $s \in \mathbb{R}$, and make the following hypotheses on the structure of its singularity.

HYPOTHESES. *There is an integer $N \geq 1$ such that for all $m = 1, \dots, N$,*

$$(2.4a) \quad \mathcal{R}_0^\alpha \mathcal{K}_0^\beta \psi^0 \in H_{s-(m-1)\nu}, \quad 0 \leq |\alpha| \leq m-1, \quad |\alpha| + |\beta| = 2m-1,$$

and

$$(2.4b) \quad \mathcal{R}_0^\alpha \mathcal{K}_0^\beta \psi^0 \in H_{s-m\nu}, \quad 0 \leq |\alpha| \leq m, \quad |\alpha| + |\beta| = 2m.$$

Note that $\mathcal{K}_0 = x - y$, and $\mathcal{R}_0 = i\partial_x - y$.

We now turn to the main result of this section.

THEOREM V. *Assume that $w(x)$ obeys (2.2), and ψ^0 satisfies the above Hypotheses with some $N \geq 1$. Then, for all t ,*

$$(2.5) \quad \mathcal{K}_t^\alpha \psi(t) \in H_{s+N(1-\nu)}, \quad \forall \alpha \in \mathbb{Z}_+^n, |\alpha| = N.$$

In particular, when $t = M\pi$, $M \in \mathbb{Z}$, we have

$$(2.6) \quad ((-1)^M x - y)^\alpha \psi(M\pi, \cdot) \in H_{s+N(1-\nu)}.$$

Since $\delta(\cdot - y) \in H_s$ for any $s < -n/2$, and $\mathcal{K}_0^j \delta(x - y) = (x^j - y^j) \delta(x - y) = 0$, $j = 1, \dots, n$, the hypotheses (2.4) are satisfied for $\psi^0(x) = \delta(x - y)$ with *arbitrary* $N \geq 1$. Theorem V then implies that $E(M\pi, \cdot, y)$ is C^∞ everywhere except at $x = (-1)^M y$. Note also that $E(M\pi, \cdot, y)$ must have a singularity at $x = (-1)^M y$. Indeed, $E(M\pi, \cdot, y)$ cannot lie in a space better than $\bigcup_{s < -n/2} H_s$, because if it does, if $E(M\pi, \cdot, y) \in H_r$ with some $r \geq n/2$, then, by Lemma 1.1, so does $E(0, \cdot, y) = \delta(\cdot - y)$, which is impossible. This proves Theorem IV.

Let us now prove Theorem V. Again, only to make the formulae shorter, we assume that $n = 1$. And again, instead of struggling through a meticulous inductive argument, we show the first two steps which comprise all the essential features of our approach.

As in the proof of Theorem I, we start with the commutator relations

$$(2.7) \quad [\mathcal{L}, \mathcal{K}_t] = -i \sin t \cdot \partial_x w(x), \quad [\mathcal{L}, \mathcal{R}_t] = -i \cos t \cdot \partial_x w(x), \quad [\mathcal{R}_t, \mathcal{K}_t] = i.$$

Let ψ be the solution of (2.1) with $\psi^0 \in H_s$. We know that $\psi \in C_{\text{loc}}(\mathbb{R} \rightarrow H_s)$. The functions $\mathcal{K}_t \psi$ and $(\mathcal{K}_t)^2 \psi$ are the solutions to the problems (see (1.9))

$$(2.8a) \quad \mathcal{L} \mathcal{K}_t \psi = -i \sin t \cdot \partial_x w(x) \cdot \psi, \quad \mathcal{K}_t \psi|_{t=0} = \mathcal{K}_0 \psi^0,$$

and

$$(2.8b) \quad \begin{aligned} \mathcal{L} (\mathcal{K}_t)^2 \psi &= -2i \sin t \cdot \partial_x w(x) \cdot \mathcal{K}_t \psi - (i \sin t)^2 \partial_x^2 w(x) \cdot \psi, \\ (\mathcal{K}_t)^2 \psi|_{t=0} &= (\mathcal{K}_0)^2 \psi^0. \end{aligned}$$

Given that $\mathcal{K}_0 \psi^0 \in H_s$ and $(\mathcal{K}_0)^2 \psi^0 \in H_{s-\nu}$, we have (apply Lemma 1.1 and use (2.2))

$$(2.9) \quad \mathcal{K}_t \psi \in C_{\text{loc}}(\mathbb{R} \rightarrow H_s), \quad (\mathcal{K}_t)^2 \psi \in C_{\text{loc}}(\mathbb{R} \rightarrow H_{s-\nu}).$$

Consider now the function $\mathcal{R}_t \circ \mathcal{K}_t \psi$. The commutator $[\mathcal{L}, \mathcal{R}_t \circ \mathcal{K}_t]$ can be written as follows:

$$\begin{aligned}
(2.10) \quad [\mathcal{L}, \mathcal{R}_t \circ \mathcal{K}_t] &= -i \cos t \cdot \partial_x w(x) \cdot \mathcal{K}_t + \mathcal{R}_t \circ (-i \sin t \cdot \partial_x w(x)) \\
&= i \cos t \cdot \partial_x w(x) \cdot \mathcal{K}_t - i \sin t \cdot \partial_x w(x) \cdot \mathcal{R}_t + \frac{1}{2} \sin 2t \cdot \partial_x^2 w(x) \\
&= -2i \cos t \cdot \partial_x w(x) \cdot \mathcal{K}_t \\
&\quad + [ix \cdot \partial_x w(x) - i\sqrt{2} \cos(t + \pi/4) \cdot y \cdot \partial_x w(x) \\
&\quad + \frac{1}{2} \sin 2t \partial_x^2 w(x)],
\end{aligned}$$

where we have used the important identity

$$(2.11) \quad \sin t \cdot \mathcal{R}_t = \cos t \cdot \mathcal{K}_t - x + \sqrt{2} \cos(t + \pi/4) \cdot y.$$

Thus, $\mathcal{R}_t \circ \mathcal{K}_t \psi$ solves the following problem:

$$\begin{aligned}
(2.12) \quad \mathcal{L} \mathcal{R}_t \circ \mathcal{K}_t \psi &= -2i \cos t \cdot \partial_x w(x) \cdot \mathcal{K}_t \psi + i B_t(w) \psi, \\
\mathcal{R}_t \circ \mathcal{K}_t \psi|_{t=0} &= \mathcal{R}_0 \circ \mathcal{K}_0 \psi^0,
\end{aligned}$$

where, of course,

$$B_t(w) = [(x - i\sqrt{2} \cos(t + \pi/4) \cdot y) \cdot \partial_x + \frac{1}{2} \sin 2t \cdot \partial_x^2] w(x).$$

In fact, all we need to know about the factor $B_t(w)$ is that it is of order $\leq \nu$ (the term $x \partial_x w(x)$ has the highest order). Since, by assumption, $\mathcal{R}_0 \circ \mathcal{K}_0 \psi^0 \in H_{s-\nu}$, we see that

$$(2.13) \quad \mathcal{R}_t \circ \mathcal{K}_t \psi \in C_{\text{loc}}(\mathbb{R} \rightarrow H_{s-\nu}).$$

The coefficient of the derivative in either (2.3a), or (2.3b), or both, does not vanish. Hence, having $\mathcal{R}_t \circ \mathcal{K}_t \psi(t) \in H_{s-\nu}$ and $\mathcal{K}_t \circ \mathcal{K}_t \psi(t) \in H_{s-\nu}$, we conclude that $\mathcal{K}_t \psi(t) \in H_{s+1-\nu}$ (see (1.3)). This proves Theorem V in the case $N = 1$.

In the case $N = 2$ we have an additional information about ψ^0 :

$$(2.14a) \quad (\mathcal{K}_0)^3 \psi^0 \in H_{s-\nu}, \quad \mathcal{R}_0 \circ (\mathcal{K}_0)^2 \psi^0 \in H_{s-\nu},$$

and

$$(2.14b) \quad (\mathcal{K}_0)^4 \psi^0 \in H_{s-2\nu}, \quad \mathcal{R}_0 \circ (\mathcal{K}_0)^3 \psi^0 \in H_{s-2\nu}, \quad (\mathcal{R}_0)^2 \circ (\mathcal{K}_0)^2 \psi^0 \in H_{s-2\nu}.$$

As before, we use the commutator identities. We have

$$\begin{aligned}
(2.15) \quad [\mathcal{L}, (\mathcal{K}_t)^3] &= -3i \sin t \cdot \partial_x w(x) \cdot (\mathcal{K}_t)^2 \\
&\quad + 3(\sin t)^2 \partial_x^2 w(x) \cdot \mathcal{K}_t + i(\sin t)^3 \partial_x^3 w(x), \\
[\mathcal{L}, \mathcal{R}_t \circ (\mathcal{K}_t)^2] &= -2i \sin t \cdot \partial_x w(x) \cdot \mathcal{R}_t \circ \mathcal{K}_t - i \cos t \cdot \partial_x w(x) \cdot (\mathcal{K}_t)^2 \\
&\quad + \frac{3}{2} \sin(2t) \partial_x^2 w(x) \cdot \mathcal{K}_t - \sin t \cdot B_t(\partial_x w(x)).
\end{aligned}$$

The first equality follows from (1.9). In deriving the second equality we have also used (2.11).

With the help of (2.15), and taking into account (2.9) and (2.13), we see that both $\mathcal{L}(\mathcal{K}_t)^3\psi$ and $\mathcal{L}(\mathcal{R}_t \circ (\mathcal{K}_t)^2\psi)$ are continuous functions of t with values in $H_{s-\nu}$. Since the initial data are in $H_{s-\nu}$ also, Lemma 1.1 says that

$$(2.16) \quad (\mathcal{K}_t)^3\psi \in H_{s-\nu}, \quad \mathcal{R}_t \circ (\mathcal{K}_t)^2\psi \in H_{s-\nu}.$$

Next, we calculate

$$\begin{aligned} [\mathcal{L}, (\mathcal{K}_t)^4] &= -4i \sin t \cdot \partial_x w(x) \cdot (\mathcal{K}_t)^3 + 6(\sin t)^2 \partial_x^2 w(x) \cdot (\mathcal{K}_t)^2 \\ &\quad + 4i(\sin t)^3 \partial_x^3 w(x) \cdot \mathcal{K}_t - (\sin t)^4 \partial_x^4 w(x), \\ [\mathcal{L}, \mathcal{R}_t \circ (\mathcal{K}_t)^3] &= -3i \sin t \cdot \partial_x w(x) \cdot \mathcal{R}_t \circ (\mathcal{K}_t)^2 - i \cos t \cdot \partial_x w(x) \cdot (\mathcal{K}_t)^3 \\ &\quad + 3(\sin t)^2 \partial_x^2 w(x) \cdot \mathcal{R}_t \circ \mathcal{K}_t + \frac{3}{2} \sin(2t) \partial_x^2 w(x) \cdot (\mathcal{K}_t)^2 \\ &\quad + 4i \cos t (\sin t)^2 \partial_x^3 w(x) \cdot \mathcal{K}_t - i(\sin t)^2 B_t(\partial_x^2 w(x)), \\ [\mathcal{L}, (\mathcal{R}_t)^2 \circ (\mathcal{K}_t)^2] &= -4i \cos t \cdot \partial_x w(x) \cdot \mathcal{R}_t \circ (\mathcal{K}_t)^2 + 2i B_t(\partial_x w(x)) \cdot \mathcal{R}_t \circ \mathcal{K}_t \\ &\quad + 4(\cos t)^2 \partial_x^2 w(x) \cdot (\mathcal{K}_t)^2 \\ &\quad - 2 \cos t \cdot [\partial_x w(x) + 2B_t(\partial_x w(x))] \cdot \mathcal{K}_t \\ &\quad - i \cdot \frac{1}{2} \sin(2t) [\partial_x^2 w(x) + B_t(\partial_x^2 w(x))]. \end{aligned}$$

These identities, together with (2.9), (2.13), (2.16) and (2.14b), lead to the conclusion that

$$(2.17) \quad (\mathcal{K}_t)^4\psi, \mathcal{R}_t \circ (\mathcal{K}_t)^3\psi, (\mathcal{R}_t)^2 \circ (\mathcal{K}_t)^2\psi \in C_{\text{loc}}(\mathbb{R} \rightarrow H_{s-2\nu}).$$

Since $(\mathcal{K}_t)^4\psi(t) \in H_{s-2\nu}$ and $\mathcal{R}_t \circ (\mathcal{K}_t)^3\psi(t) \in H_{s-2\nu}$, we have, invoking again (1.3),

$$(2.18a) \quad (\mathcal{K}_t)^3\psi(t) \in H_{s+1-2\nu}.$$

On the other hand, since $\mathcal{K}_t \circ \mathcal{R}_t \circ (\mathcal{K}_t)^2\psi(t) \in H_{s-2\nu}$ (see (2.7) and (2.17)), and $(\mathcal{R}_t)^2 \circ (\mathcal{K}_t)^2\psi(t) \in H_{s-2\nu}$, we have

$$(2.18b) \quad \mathcal{R}_t \circ (\mathcal{K}_t)^2\psi(t) \in H_{s+1-2\nu}.$$

For the same reason as above, (2.18a) and (2.18b) allow to improve the regularity of $(\mathcal{K}_t)^2\psi(t)$, and we obtain

$$(2.19) \quad (\mathcal{K}_t)^2\psi(t) \in H_{s+2-2\nu}.$$

This proves the theorem in the case $N = 2$. To handle the general case, one has to use induction. However, the justification of the inductive step uses exactly the same ideas as the ones we have just used to pass from $N = 1$ to $N = 2$. We skip the formal argument.

3. Representation of the kernel

In this section we prove Theorem III. We assume that the perturbation, $w(x)$, is real-valued, infinitely differentiable, and satisfies the conditions

$$(3.1) \quad |\partial_x^\alpha w(x)| = o(1) \quad \text{as } |x| \rightarrow \infty, \quad \forall \alpha \in \mathbb{Z}_+^n, \quad |\alpha| \geq 2.$$

With the quantum Hamiltonian

$$(3.2) \quad H = -\frac{1}{2}\Delta + \frac{1}{2}|x|^2 + w(x),$$

we associate the classical Hamilton function

$$H(q, p) = \frac{1}{2}|p|^2 + \frac{1}{2}|q|^2 + w(q).$$

Denote by $q(t, y, \xi)$, $p(t, y, \xi)$ the solution of the classical Hamiltonian system

$$(3.3a) \quad \begin{cases} \frac{\partial}{\partial t} q = p, \\ \frac{\partial}{\partial t} p = q - \frac{\partial}{\partial q} w(q), \end{cases}$$

subject to the initial conditions

$$(3.3b) \quad q(0, y, \xi) = y, \quad p(0, y, \xi) = \xi.$$

As shown in [Fujiwara, 1979], under even weaker assumptions on w , there exists $\tau_* > 0$ so that, for every $t \in (0, \tau_*]$ and every $y \in \mathbb{R}^n$, the mapping $\mathbb{R}^n \ni \xi \mapsto q(t, y, \xi) \in \mathbb{R}^n$ is a diffeomorphism. Hence, given $x, y \in \mathbb{R}^n$ and $t \in (0, \tau_*]$, there exists a unique ξ such that $x = q(t, y, \xi)$. One then defines the classical action as follows:

$$(3.4) \quad S(t, x, y) = \int_0^t \left[\frac{1}{2}|p(s, y, \xi)|^2 - \frac{1}{2}|q(s, y, \xi)|^2 - w(q(s, y, \xi)) \right] ds.$$

Fujiwara also showed that, when $0 < t \leq \tau_*$, the function $S(t, x, y)$ is smooth and, moreover,

$$(3.5) \quad S(t, x, y) = \frac{|x - y|^2}{2t} + t\Phi(t, x, y),$$

where $\Phi(t, x, y)$ satisfies the estimates

$$(3.6) \quad |\partial_x^\alpha \partial_y^\beta \Phi(t, x, y)| \leq \varkappa_{\alpha, \beta}, \quad \forall \alpha, \beta, \quad |\alpha + \beta| \geq 2,$$

with constants $\varkappa_{\alpha, \beta}$ independent of $t \in (0, \tau_*]$ and x, y . The regularity in t can be derived from the eikonal equation satisfied by $S(t, x, y)$,

$$\frac{\partial}{\partial t} S(t, x, y) + \frac{1}{2} \left| \frac{\partial S}{\partial x}(t, x, y) \right|^2 + \frac{1}{2}|x|^2 + w(x) = 0,$$

and the above estimates on the spatial derivatives.

In what follows, we will choose τ_* sufficiently small. Then we will have, in particular, the estimate

$$(3.7) \quad \inf_{|y| \leq R} \left| \frac{\partial}{\partial y} S(t, x, y) \right| \geq c(R)|x|,$$

for all sufficiently large x .

We need the basic result of [Fujiwara, 1980] on the structure of the fundamental solution $E(t, x, y)$ of the Schrödinger equation with the Hamiltonian (3.2).

THEOREM 3.1. *For $t \in (0, \tau_*]$,*

$$(3.8) \quad E(t, x, y) = a(t, x, y) e^{iS(t, x, y)},$$

where $a(t, x, y)$ is a smooth function for which the following estimates hold provided t stays away from 0:

$$\sup_{\substack{0 < \varepsilon \leq t < \tau_* \\ x, y \in \mathbb{R}^n}} |\partial_t^l \partial_x^\alpha \partial_y^\beta a(t, x, y)| \leq c_{l, \alpha, \beta}(\varepsilon), \quad \forall l = 0, 1, 2, \dots, \forall \alpha, \beta \in \mathbb{Z}_+^n.$$

We are now in a position to prove Theorem III. Choose an arbitrary (large) $T > 0$ and a sufficiently small $\varepsilon \in (0, \pi/2)$. Define $\mathfrak{T} = \{t : 0 < t \leq T, \text{dist}(t, \pi\mathbb{Z}) \geq \varepsilon\}$.

We will construct the fundamental solution $E(t, x, y)$ for $t \in \mathfrak{T}$ by glueing together Fujiwara's local representations.

We can always choose the nodal points $0 = t_0 < t_1 < \dots < t_M$ so that $t_j \in \mathfrak{T}$, $j = 1, \dots, M$, and, for every $t \in \mathfrak{T}$, one has $t_j \leq t < t_{j+1}$ and $s = t - t_j < \tau_*/2$. (After the proof of Proposition 3.2 below, we discuss in more detail the choice of t_j 's.)

Writing e^{-itH} as a product,

$$(3.9) \quad e^{-itH} = e^{-i(t-t_j)H} \dots e^{-i(t_1-t_0)H},$$

we see that each of the factors $e^{-i(t_{k+1}-t_k)H}$ and $e^{-i(t-t_j)H}$ is an integral operator with a kernel that has Fujiwara's representation (3.8). To construct $E(t, x, y)$, we take the composition of these integral operators and find its kernel. Thus, we need the following result.

PROPOSITION 3.2. *Let \mathcal{E} be an integral operator with kernel*

$$(3.10) \quad \mathcal{E}(x, y) = b(x, y) e^{i\sigma(x, y)},$$

where $b(\cdot, \cdot)$ is a smooth function, bounded with all its derivatives; $\sigma(\cdot, \cdot)$ is also smooth, and its derivatives obey the estimates

$$(3.11a) \quad |\partial_x^\alpha \partial_y^\beta \sigma(x, y)| \leq c_{\alpha, \beta}, \quad |\alpha + \beta| \geq 2.$$

Let ε be given so that

$$(3.12) \quad 0 < \varepsilon < \min \left\{ \frac{\tau_*}{4}, \frac{1}{4\pi\tau_*\varkappa_{0,2}} \right\},$$

where $\varkappa_{0,2}$ is the maximal of all constants $\varkappa_{\alpha,\beta}$ in (3.6) with $\alpha = 0$ and $|\beta| = 2$. Assume that there exist $\theta > 0$ and $\varrho > 0$ such that

$$(3.11b) \quad \begin{aligned} &1) \text{ dist}(\theta, \pi\mathbb{Z}) \geq \varepsilon, \\ &2) \text{ for all } x \text{ and } y \text{ with } |x|^2 + |y|^2 > \varrho^2, \\ &\sigma(x, y) = S(\theta, x, y), \end{aligned}$$

where $S(\theta, x, y)$ is defined as in (3.4). We assume that ϱ is sufficiently large, the lower bound on its size is determined by τ_* , $\varkappa_{0,2}$, and ε , as in Lemma A.5 of Appendix. Given s such that

$$(3.13) \quad 0 < s < \tau_*, \quad \left| \cot \theta + \frac{1}{s} \right| \geq \frac{1}{4\varepsilon}, \quad \text{dist}(s + \theta, \pi\mathbb{Z}) \geq \varepsilon,$$

the product $\mathcal{J} = e^{-isH}\mathcal{E}$ is an integral operator with kernel $\mathcal{J}(x, y)$ of the form

$$(3.14) \quad \mathcal{J}(x, y) = b_s(x, y) e^{i\sigma_s(x, y)},$$

where $b_s(\cdot, \cdot)$ is smooth and bounded with all its derivatives, $\sigma_s(\cdot, \cdot)$ satisfies (3.11a) (with probably different bounds $c_{\alpha,\beta}$), and

$$(3.15) \quad \sigma_s(x, y) = S(s + \theta, x, y), \quad \forall x, y : |x|^2 + |y|^2 > \varrho^2.$$

For all t sufficiently close to s , the function $b_t(x, y)$ and its derivatives remain uniformly bounded, and the estimates (3.11a) hold for $\sigma_t(x, y)$ with, perhaps, larger constants $c_{\alpha,\beta}$. Also, $b_t(x, y)$ and $\sigma_t(x, y)$ are infinitely differentiable in t when t stays within a sufficiently small neighborhood of s .

A critical reader has probably noticed that we use $S(\theta, x, y)$ without smallness assumption on θ . It turns out, however, that for large, non-resonant θ , the action $S(\theta, x, y)$ is also well defined if $|x|^2 + |y|^2$ is sufficiently large. We establish this in Appendix, where we study the properties of $S(t, x, y)$. The results of Appendix are heavily used in the proof below.

PROOF OF PROPOSITION 3.2. Formally, $\mathcal{J}(x, y)$ can be written as an integral,

$$(3.16) \quad \mathcal{J}(x, y) = \int a(s, x, z) e^{iS(s, x, z)} b(z, y) e^{i\sigma(z, y)} dz,$$

where $a(s, x, z) e^{iS(s, x, z)}$ is the kernel of e^{-isH} given by Fujiwara's construction. Our goal is to show that the integral in (3.16) defines a C^∞ function that can be written in the form (3.14).

By assumption, $\theta, s + \theta \in \mathfrak{T}$. Lemma A.7 assures that $S(t, x, y)$ is a (well defined) smooth function on the set $\mathfrak{T} \times B_{\geq \varrho}$, where $B_{\geq \varrho} = \{(x, y) \in \mathbb{R}^{2n} : |x|^2 + |y|^2 \geq \varrho^2\}$, and $\varrho = \varrho(\varepsilon)$ is large enough (as in Lemma A.5). Note that our assumptions (3.12) and (3.13) are needed for Lemma A.7.

Choose a cut-off function $\chi_1^< \in C_0^\infty(\mathbb{R}^n \times \mathbb{R}^n)$ so that $\chi_1^< \geq 0$, $\chi_1^<(z, y) = 1$ if $|z|^2 + |y|^2 \leq 1$, and $\chi_1^<(z, y) = 0$ if $|z|^2 + |y|^2 \geq 2$. For $r > 0$, define $\chi_r^<(z, y) = \chi_1^<(z/r, y/r)$ and $\chi_r^>(z, y) = 1 - \chi_r^<(z, y)$.

We write the integral (3.14) as a sum of two integrals, $J(x, y) = J^<(x, y) + J^>(x, y)$, where

$$(3.17a) \quad J^<(x, y) = \int a(s, x, z) e^{iS(s, x, z)} \chi_\varrho^<(z, y) b(z, y) e^{i\sigma(z, y)} dz,$$

$$(3.17b) \quad J^>(x, y) = \int a(s, x, z) e^{iS(s, x, z)} \chi_\varrho^>(z, y) b(z, y) e^{i\sigma(z, y)} dz.$$

Because of (3.5)–(3.7), integration by parts shows that $J^<(x, y)$ is a rapidly decreasing function on $\mathbb{R}^n \times \mathbb{R}^n$. We, therefore, may ignore it.

In view of (3.11b), the second integral takes the form

$$(3.17c) \quad J^>(x, y) = \int a(s, x, z) b(z, y) \chi_\varrho^>(z, y) e^{i[S(s, x, z) + S(\theta, z, y)]} dz.$$

As we show in Lemma A.7(b) of Appendix,

$$\left| \frac{\partial}{\partial z} [S(s, x, z) + S(\theta, z, y)] \right| \geq \frac{1}{8\varepsilon} |z|,$$

for all sufficiently large $|z|$. Then we can integrate by parts in (3.17c) and show that $J^>(x, y)$ is C^∞ in x and y .

Now, we take ϱ_1 as defined in Lemma A.7(d), and write $J^>(x, y)$ as a sum of $\chi_{\varrho_1}^<(x, y) J^>(x, y)$ and $\chi_{\varrho_1}^>(x, y) J^>(x, y)$. The first being a $C_0^\infty(\mathbb{R}^n \times \mathbb{R}^n)$ function, we ignore it and focus on the second. We treat the integral

$$(3.17d) \quad J^{>>}(x, y) = \int \chi_{\varrho_1}^>(x, y) a(s, x, z) b(z, y) \chi_\varrho^>(z, y) e^{i[S(s, x, z) + S(\theta, z, y)]} dz$$

with the stationary phase method developed in [Asada & Fujiwara, 1978]. Since, on the support of the integrand, $|x|^2 + |y|^2 \geq \varrho_1^2$ and $|z|^2 + |y|^2 \geq \varrho^2$, Lemma A.7(d) tells us that there exists a unique stationary point z_* of the phase function

$$\Phi_{s, \theta, x, y}(z) = S(s, x, z) + S(\theta, z, y),$$

and $S(s, x, z_*) + S(\theta, z_*, y) = S(s + \theta, x, y)$. Part (f) of Lemma A.7 shows that the Hessian of $\Phi(z)$ is non-degenerate (see (A.29)). In addition, all partial derivatives of order two and higher of $\Phi_{s, \theta, x, y}(z)$ with respect to x, y , and z are bounded. Also, as we prove in Lemma A.7(e), the first derivatives of $\Phi_{s, \theta, x, y}(z)$ are bounded from below. Thus, all the conditions of Lemma 3.2 of [Asada & Fujiwara, 1978] are fulfilled. We apply their result to $J^{>>}(x, y)$ and obtain the

desired representation for $J^{\gg}(x, y)$ and, hence, for $J(x, y)$. The regularity of $b_t(x, y)$ and $\sigma_t(x, y)$ in t , for t close to s , also follows from the above arguments and Proposition 3.1. \square

On the choice of the nodal points t_j . Let $T > 0$ and ε be fixed. We assume that ε obeys (3.12) and, in addition, $\varepsilon < \pi/2$ and

$$(3.18) \quad \frac{\tan \varepsilon}{\varepsilon} < \frac{4}{3}.$$

To be able to use Proposition 3.2, we must choose the nodal points $t_1, \dots, t_M \in \mathfrak{T}$ appropriately. This means that the following conditions must be satisfied:

$$t_{j+1} - t_j < \tau_*, \quad j = 0, \dots, M-1,$$

and also (see (3.13)),

$$\left| \cot t_j + \frac{1}{t - t_j} \right| \geq \frac{1}{4\varepsilon} \quad \text{if } t_j < t \leq t_{j+1}, \quad t \in \mathfrak{T}.$$

We claim that they are satisfied if we take as nodal points all $\theta \in \mathfrak{T}$ of the form $m\pi \pm \varepsilon$, and, in addition, inside each interval $(m\pi + \varepsilon, (m+1)\pi - \varepsilon)$, all the points $m\pi + \varepsilon + l\varepsilon/2$ with integer $l > 0$. Thus, we have to consider two cases: a) $t - t_j \leq \varepsilon/2$, and b) $t = t_{j+1} = t_j + 2\varepsilon$. In the case a) we have

$$\left| \cot t_j + \frac{1}{t - t_j} \right| \geq \frac{1}{t - t_j} - |\cot t_j| \geq \frac{2}{\varepsilon} - \cot \varepsilon \stackrel{(3.18)}{\geq} \frac{1}{4\varepsilon}.$$

In the case b) we have, for some integer m ,

$$\left| \cot t_j + \frac{1}{t - t_j} \right| = \left| \cot(m\pi - \varepsilon) + \frac{1}{2\varepsilon} \right| \stackrel{(3.18)}{=} \cot \varepsilon - \frac{1}{2\varepsilon} \stackrel{(3.18)}{\geq} \frac{1}{4\varepsilon}.$$

One final remark to complete the proof of Theorem III: The small variation of t in e^{-itH} affects only the leftmost factor on the right side of (3.9). Applying Proposition 3.2 and taking into account the compactness of the interval $[k\pi + \varepsilon, (k+1)\pi - \varepsilon]$, we obtain the estimates (0.11).

A. Appendix

Consider a Hamiltonian of the form

$$(A.1) \quad H(q, p) = \frac{1}{2}|p|^2 + \frac{1}{2}|q|^2 + w(q), \quad q, p \in \mathbb{R}^n,$$

where $w(q)$ is a smooth function satisfying the conditions

$$(A.2) \quad |\partial_x^\alpha w(q)| = o(1) \quad \text{as } |q| \rightarrow \infty, \quad |\alpha| \geq 2.$$

Let $q(t, y, \eta)$, $p(t, y, \eta)$ denote the solution of the classical Hamiltonian system

$$(A.3a) \quad \begin{cases} \frac{\partial}{\partial t} q = p, \\ \frac{\partial}{\partial t} p = q - \frac{\partial}{\partial q} w(q), \end{cases}$$

subject to the initial conditions

$$(A.3b) \quad q(0, y, \eta) = y, \quad p(0, y, \eta) = \eta.$$

The assumption (A.2) guarantees the existence and uniqueness of the global trajectory $(q(t, y, \eta), p(t, y, \eta))$, $-\infty < t < \infty$, for any choice of the initial data $(y, \eta) \in \mathbb{R}^{2n}$.

Note that $q(t, y, \eta)$, $p(t, y, \eta)$ satisfy the following integral equations:

$$(A.4) \quad \begin{cases} q(t, y, \eta) = \cos t \cdot y + \sin t \cdot \eta - \int_0^t \sin(t-s) \frac{\partial}{\partial q} w(q(s, y, \eta)) ds, \\ p(t, y, \eta) = -\sin t \cdot y + \cos t \cdot \eta - \int_0^t \cos(t-s) \frac{\partial}{\partial q} w(q(s, y, \eta)) ds. \end{cases}$$

We pick and fix, for the rest of this section, an arbitrary $T > 0$ and a sufficiently small $\varepsilon > 0$. Until Lemma A.7 below, it suffices to have $\varepsilon < \pi/2$. However, for Lemma A.7, we require that $(\tan \varepsilon)/\varepsilon < 4/3$, and, in addition, $\varepsilon < \min\{\tau_*/4, 1/(4\pi\tau_*\varkappa_{0,2})\}$, where the numbers τ_* and $\varkappa_{0,2}$ are borrowed from Fujiwara's construction of the local-in-time fundamental solution (see [Fujiwara 1979] and Remark A.6 below).

Denote by \mathfrak{T} the set

$$\mathfrak{T} = \{t : 0 < t \leq T, |t - m\pi| \geq \varepsilon, \forall m \in \mathbb{Z}\}.$$

LEMMA A.1. *For every $r' > 0$ there exists $C = C(r') > 0$ such that*

$$(A.5) \quad (|y|^2 + |\eta|^2)^{1/2} \cdot |\{t \in \mathfrak{T} : |q(t, y, \eta)| \leq r'\}| \leq C,$$

where $|\{\dots\}|$ stands for the measure of the set $\{\dots\}$.

Before we turn to the proof of this lemma, we mention a few simple properties of $w(q)$ and $H(q, p)$ that follow from (A.2), which we need here and later on.

LEMMA A.2. *For every δ , $0 < \delta < 1/2$, there exist $r_\delta > 0$ and $C_\delta > 0$ such that*

- (i) $|w(q)| + |q| \cdot |\partial w(q)/\partial q| \leq \delta |q|^2 + C_\delta$ if $|q| > r_\delta$;
- (ii) $|\partial^2 w(q)/\partial q^2| \leq \delta$ if $|q| > r_\delta$;
- (iii) $(1 - \delta)(\frac{1}{2}|q|^2 + \frac{1}{2}|p|^2) \leq H(q, p) \leq (1 + \delta)(\frac{1}{2}|q|^2 + \frac{1}{2}|p|^2)$
if $\sqrt{|q|^2 + |p|^2} > r_\delta$.

PROOF OF LEMMA A.1. Due to the conservation of energy and statement (iii) of Lemma A.2, we may assume in the proof of (A.5) that $|y| \leq r'$ and, at the same time, $r^2 = |y|^2 + |\eta|^2$ is sufficiently large.

Consider the quantity $u(t) = |q(t, y, \eta)|^2$. It is easy to check that $u(t)$ satisfies the equation

$$\frac{d^2}{dt^2}u(t) + 4u(t) = 4H(y, \eta) - 4w(q) - 2q \frac{\partial w}{\partial q}.$$

We choose a sufficiently small $\delta > 0$ and, assuming that $|y|^2 + |\eta|^2 \geq r_\delta^2$, estimate the right hand side from below by $2(1 - \delta)r_\delta^2 - 4\delta u(t) - 4C_\delta$ (see Lemma A.2). Thus, we get an inequality

$$(A.6) \quad \frac{d^2}{dt^2}u(t) + 4(1 + \delta)u(t) \geq 2(1 - \delta)r_\delta^2 - 4C_\delta.$$

Let $v(t)$ be the solution of the equation

$$(A.7a) \quad \frac{d^2}{dt^2}v(t) + 4(1 + \delta)v(t) = 2(1 - \delta)r_\delta^2 - 4C_\delta,$$

subject to the same initial conditions as $u(t)$, i.e.,

$$(A.7b) \quad v(0) = |y|^2, \quad \frac{d}{dt}v(0) = 2y \cdot \eta.$$

The standard comparison theorem for the solutions of second-order equations [Kamke, Theorem 24.3] tells that $u(t) \geq v(t)$ for all $t > 0$. Now, $v(t)$ is known explicitly, namely,

$$v(t) = \cos(\lambda t) \cdot |y|^2 + \frac{1}{\lambda} \sin(\lambda t) \cdot 2y\eta + \frac{1 - \cos(\lambda t)}{\lambda^2} [2(1 - \delta)r_\delta^2 - 4C_\delta],$$

where $\lambda = 2\sqrt{1 + \delta}$. Hence,

$$(A.8a) \quad \cos(\lambda t) \cdot |y|^2 + \frac{1}{\lambda} \sin(\lambda t) \cdot 2y\eta + \frac{1 - \cos(\lambda t)}{\lambda^2} [2(1 - \delta)r_\delta^2 - 4C_\delta] \leq u(t).$$

If $u(t) \leq (r')^2$, then we should have

$$(A.8b) \quad \cos(\lambda t) \cdot |y|^2 + \frac{1}{\lambda} \sin(\lambda t) \cdot 2y\eta + \frac{1 - \cos(\lambda t)}{\lambda^2} [2(1 - \delta)r_\delta^2 - 4C_\delta] \leq (r')^2.$$

We note that $|\cos(\lambda t)| \cdot |y|^2 \leq (r')^2$. Also,

$$\begin{aligned} \left| \frac{1}{\lambda} \sin(\lambda t) \cdot 2y\eta \right| &= \left| \cos\left(\frac{\lambda t}{2}\right)y \cdot \left| \frac{2}{\lambda} \sin\left(\frac{\lambda t}{2}\right)\eta \right| \right| \\ &\leq \frac{1}{4\delta} \cdot \cos^2\left(\frac{\lambda t}{2}\right) |y|^2 + \delta \cdot \frac{4}{\lambda^2} \sin^2\left(\frac{\lambda t}{2}\right) |\eta|^2 \\ &\leq \frac{1}{4\delta} (r')^2 + \delta \cdot \frac{4}{\lambda^2} \sin^2\left(\frac{\lambda t}{2}\right) r_\delta^2. \end{aligned}$$

Thus, (A.8b) implies the estimate

$$\frac{4}{\lambda^2} \sin^2 \left(\frac{\lambda t}{2} \right) (1 - 2\delta) r_\delta^2 \leq \left(2 + \frac{1}{4\delta} \right) (r')^2 + \frac{8C_\delta}{\lambda^2},$$

from which (A.5) follows. \square

LEMMA A.3. *For every $\varepsilon_1 > 0$ there exists $R_1 = R_1(\varepsilon_1) > 0$ such that the following estimates hold:*

$$(A.9a) \quad \left\| \frac{\partial}{\partial \eta} q(t, y, \eta) - \sin t \cdot \mathbf{1} \right\| \leq \varepsilon_1, \quad \forall t \in \mathfrak{T},$$

$$(A.9b) \quad \left\| \frac{\partial}{\partial y} q(t, y, \eta) - \cos t \cdot \mathbf{1} \right\| \leq \varepsilon_1, \quad \forall t \in \mathfrak{T},$$

$$(A.9c) \quad \left\| \frac{\partial}{\partial \eta} p(t, y, \eta) - \cos t \cdot \mathbf{1} \right\| \leq \varepsilon_1, \quad \forall t \in \mathfrak{T},$$

when $|y|^2 + |\eta|^2 \geq R_1^2$.

PROOF. We will prove the first estimate, the other two are proved similarly.

Differentiating the first of the equations (A.4) with respect to η we obtain

$$(A.10a) \quad \frac{\partial}{\partial \eta} q(t, y, \eta) = \sin t \cdot \mathbf{1} - \int_0^t \sin(t-s) \frac{\partial^2}{\partial q \partial q} w(q(s, y, \eta)) \frac{\partial}{\partial \eta} q(s, y, \eta) ds.$$

Denoting by K the supremum of $|\partial^2 w(q)/\partial q^2|$, and applying Gronwall's inequality to (A.10a), we get the estimate

$$\left\| \frac{\partial}{\partial \eta} q(t, y, \eta) \right\| \leq 1 + K \int_0^t \left\| \frac{\partial}{\partial \eta} q(s, y, \eta) \right\| ds \leq e^{Kt} \leq e^{KT}.$$

Hence,

$$(A.10b) \quad \left\| \frac{\partial}{\partial \eta} q(t, y, \eta) - \sin t \cdot \mathbf{1} \right\| \leq e^{KT} \int_0^t \left\| \frac{\partial^2}{\partial q \partial q} w(q(s, y, \eta)) \right\| ds.$$

In view of (A.2), there exists r' such that

$$\left\| \frac{\partial^2}{\partial q \partial q} w(q) \right\| \leq \frac{1}{2} \varepsilon_1 e^{-KT} T^{-1} \quad \text{for } |q| \geq r'.$$

By Lemma A.1, there exists C_0 such that the time $q(t, y, \eta)$ spends inside the ball of radius r' is less than $C_0(|y|^2 + |\eta|^2)^{-1/2}$. We can now choose R_1 to be the maximal of r' and $2C_0 K e^{KT} \varepsilon_1^{-1}$. Indeed, if $|y|^2 + |\eta|^2 \geq R_1^2$, then the interval of integration in (A.10b) breaks into two parts: one consists of those t for which $|q(t, y, \eta)| \geq r'$, and the other has measure less than $\frac{1}{2} K^{-1} e^{-KT} \varepsilon_1$. Both integrals turn out to be less than $\frac{1}{2} \varepsilon_1 e^{-KT}$, which results in the desired estimate (A.9a). \square

For $t \in \mathfrak{T}$, consider the mapping

$$(A.11) \quad F_t : (y, \eta) \mapsto (y, q(t, y, \eta)).$$

Denote by J_t the Jacobian of F_t , and by A_t the matrix

$$A_t = \begin{pmatrix} \mathbf{1} & \mathbf{0} \\ \cos t \cdot \mathbf{1} & \sin t \cdot \mathbf{1} \end{pmatrix}.$$

If we take $\varepsilon_1 \leq \sin \varepsilon / (8\pi)$ and choose R_1 according to Lemma A.3, then we have

$$(A.12a) \quad \|J_t - A_t\| \leq \frac{\sin \varepsilon}{4\pi},$$

for all $t \in \mathfrak{T}$ and all y and η such that $|y|^2 + |\eta|^2 \geq R_1^2$. On the other hand, evidently,

$$(A.12b) \quad \|A_t^{-1}\| \leq \frac{2}{\sin \varepsilon}, \quad \|A_t\| \leq \sqrt{2},$$

for all $t \in \mathfrak{T}$.

The estimates (A.12) will allow us to show that F_t is a diffeomorphism of the set $B_{\geq R} = \{|y|^2 + |\eta|^2 \geq R^2\}$ onto its image, for some $R \geq R_1$. To this end we need the following abstract result.

We change the notation so that x , temporarily, is a vector in \mathbb{R}^N , for some $N > 0$. We will make use of the following notation:

$$B_{\leq R} = \{x : |x| \leq R\}, \quad B_{\geq R} = \{x : |x| \geq R\}.$$

LEMMA A.4. *Let F be a smooth mapping of \mathbb{R}^N into itself. Assume that there exists a non-singular matrix A such that*

$$(A.13) \quad \left\| \frac{\partial F}{\partial x}(x) - A \right\| \leq (\pi \|A^{-1}\|)^{-1}, \quad \forall x \in B_{\geq R}.$$

Then:

- (i) F is a diffeomorphism from $B_{\geq R}$ to its image.
- (ii) The following inclusion holds: $F(B_{\geq R}) \supset B_{\geq \varrho}$, where

$$(A.14) \quad \varrho = 36M(1 + \pi \|A^{-1}\| \cdot \|A\|), \quad M = \sup_{|x|=R} |F(x) - Ax|.$$

- (iii) In addition, $|F(x)| \geq |x|/(2\|A^{-1}\|)$ provided $|x| \geq 6M\|A^{-1}\|$.
- (iv) If $F(x_0) = 0$ for some $x_0 \in B_{\geq R}$, then

$$|F(x)| \geq (2\|A^{-1}\|)^{-1}|x - x_0|$$

for all $x \in B_{\geq R}$.

PROOF. By assumption, the matrix $\partial F(x)/\partial x$ is the sum of the non-singular matrix A and a matrix whose norm is not greater than $\pi^{-1}\|A\|$ (see (A.13)). The implicit function theorem then proves part (i).

For $z \in B_{\geq R}$, set $\hat{z} = z/|z|$. Obviously,

$$F(z) - F(\hat{z}) = \int_0^1 \frac{\partial}{\partial x} F(\lambda z + (1 - \lambda)\hat{z}) d\lambda \cdot (z - \hat{z}).$$

Therefore,

$$(A.15) \quad |F(z) - F(\widehat{z}) - A(z - \widehat{z})| \leq (\pi \|A^{-1}\|)^{-1} |z - \widehat{z}|.$$

Using this estimate and taking into account the definition of M (see (A.14)), we obtain

$$|F(z) - Az| \leq |F(\widehat{z}) - A\widehat{z}| + \frac{|z - \widehat{z}|}{\pi \|A^{-1}\|} \leq M + \frac{|z|}{\pi \|A^{-1}\|}.$$

Since $|Az| \geq \|A^{-1}\|^{-1}|z|$, it follows that

$$|F(z)| \geq \|A^{-1}\|^{-1}|z| - M - \frac{|z|}{\pi \|A^{-1}\|} \geq \frac{2|z|}{3\|A^{-1}\|} - M \geq \frac{|z|}{2\|A^{-1}\|},$$

provided $|z| \geq 6\|A^{-1}\|M$. This proves (iii).

To prove (ii), we modify $F(x)$ inside the ball $B_{\leq 3R/\delta}$, where $\delta < 1$ will be chosen later. Take a cut-off function $\phi \in C_0^\infty(\mathbb{R}^N)$ such that $\phi(x) = 1$ for $|x| \geq 3R$, $\phi(x) = 0$ for $|x| \leq 3/(2R)$ and $|\nabla\phi(z)| \leq \frac{21}{30}R^{-1}$. For $0 < \delta < 1$, we define $F_\delta(x)$ for all $x \in \mathbb{R}^N$ as follows:

$$F_\delta(x) = \begin{cases} F(x), & |x| \geq 3R/\delta, \\ \phi(\delta x)F(x) + (1 - \phi(\delta x))Ax, & 3R/\delta \geq |x| \geq 3R/(2\delta), \\ Ax, & |x| \leq 3R/(2\delta). \end{cases}$$

So defined, $F_\delta(\cdot)$ is infinitely differentiable. For all $x \in \mathbb{R}^N$ satisfying $3R/(2\delta) \leq |x| \leq 3R/\delta$, we have

$$\begin{aligned} \left\| \frac{\partial F_\delta}{\partial x}(x) - A \right\| &\leq \left\| \phi(\delta x) \left(\frac{\partial F}{\partial x}(x) - A \right) \right\| + \|\delta(\nabla\phi(\delta x)) \cdot (F(x) - Ax)\| \\ &\stackrel{(A.15)}{\leq} \frac{1}{\pi \|A^{-1}\|} + \frac{21}{30R} \delta \left(|F(\widehat{x}) - A\widehat{x}| + \frac{|x|}{\pi \|A^{-1}\|} \right), \end{aligned}$$

where $\widehat{x} = x/|x|$. Using the definition of M and replacing $|x|$ by $3R/\delta$, we obtain the estimate

$$\left\| \frac{\partial F_\delta}{\partial x}(x) - A \right\| \leq \frac{31}{10\pi \|A^{-1}\|} + \frac{21\delta M}{30R}.$$

Note that if

$$(A.16) \quad \delta < \frac{15R}{21M} \left(1 - \frac{31}{10\pi} \right) \frac{1}{\|A^{-1}\|},$$

then

$$\frac{21\delta M}{30R} < \frac{1}{2} \left(1 - \frac{31}{10\pi} \right) \frac{1}{\|A^{-1}\|},$$

and we have

$$\left\| \frac{\partial F_\delta}{\partial x} - A \right\| < \varepsilon \|A^{-1}\|^{-1},$$

where $\varepsilon = \frac{1}{2} \left(1 + \frac{31}{10\pi} \right) < 1$. Hence, F_δ is a global diffeomorphism of \mathbb{R}^N .

Now, we choose a δ which satisfies (A.16) as follows:

$$\delta = \min \left\{ \frac{R}{35\pi\|A^{-1}\|M}, 1 \right\}.$$

Then, clearly,

$$F(B_{\geq R}) \supset F_{\delta}(B_{\geq 3R/\delta}) = \mathbb{R}^N \setminus F_{\delta}(B_{< 3R/\delta}).$$

At the same time, for $|x| \leq 3R/\delta$ we have

$$\begin{aligned} |F_{\delta}(x)| &\leq |Ax| + \phi(\delta x)|F(x) - Ax| \leq |Ax| + M + \frac{|x|}{\pi\|A^{-1}\|} \\ &\leq \left(\|A\| + \frac{1}{\pi\|A^{-1}\|} \right) \frac{3}{R} \delta + M = M \left\{ \left(\|A\| + \frac{1}{\pi\|A^{-1}\|} \right) 35\pi\|A^{-1}\| + 1 \right\} \\ &\leq 36M(1 + \pi\|A\| \cdot \|A^{-1}\|). \end{aligned}$$

This proves (ii).

Finally, if $F(x_0) = 0$ for some $x_0 \in B_{\geq R}$, and $x \in B_{\geq R}$, then we have

$$F(x) - A(x - x_0) = \int_0^1 \left(\frac{\partial F}{\partial x}(\gamma(\lambda)) - A \right) \cdot \dot{\gamma}(\lambda) d\lambda,$$

where $\gamma(\lambda)$ is a semi-circle in $B_{\geq R}$ of radius $|x - x_0|/2$, connecting $x_0 = \gamma(0)$ with $x = \gamma(1)$. Estimating the integral, we obtain

$$\begin{aligned} |F(x) - A(x - x_0)| &\leq \int_0^1 \left| \frac{\partial F}{\partial x}(\gamma(\lambda)) - A \right| \cdot |\dot{\gamma}(\lambda)| d\lambda \\ &\stackrel{(A.13)}{\leq} (\pi\|A^{-1}\|)^{-1} \pi \frac{|x - x_0|}{2} = (2\|A^{-1}\|)^{-1} |x - x_0|. \end{aligned}$$

Therefore,

$$|F(x)| \geq |A(x - x_0)| - (2\|A^{-1}\|)^{-1} |x - x_0| \geq (2\|A^{-1}\|)^{-1} |x - x_0|.$$

The proof of part (iv) and the lemma is complete. \square

Returning to the mapping $F_t : \mathbb{R}^{2n} \rightarrow \mathbb{R}^{2n}$ defined in (A.11), we prove the following result.

LEMMA A.5. *There exists $R > 0$ such that the following holds true.*

- (a) *For every $t \in \mathfrak{T}$, the mapping $F_t : (y, \eta) \mapsto (y, q(t, y, \eta))$ is a diffeomorphism of the set $B_{\geq R} = \{|y|^2 + |\eta|^2 \geq R^2\}$ onto $F_t(B_{\geq R})$.*
- (b) *For every $t \in \mathfrak{T}$, $F_t(B_{\geq R}) \supset B_{\geq \varrho}$, where*

$$(A.17) \quad \varrho = 108(1 + 2\sqrt{2}\pi)R/\sin \varepsilon.$$

- (c) *For every $(y, x) \in B_{\geq \varrho}$ there exists a unique $\eta \in \mathbb{R}^n$ such that $F_t(y, \eta) = (y, x)$, and so the inverse mapping $F_t^{-1} : B_{\geq \varrho} \rightarrow B_{\geq R} \subset \mathbb{R}^{2n}$ is well*

defined. The corresponding mapping $(t, y, x) \mapsto (y, \eta)$ is smooth on $\mathfrak{T} \times B_{\geq \varrho}$.

(d) For every $t \in \mathfrak{T}$,

$$(A.18) \quad |F_t(y, \eta)| \geq \frac{\sin \varepsilon}{4} \sqrt{|y|^2 + |\eta|^2} \quad \text{if } \sqrt{|y|^2 + |\eta|^2} \geq \frac{36}{\sin \varepsilon} R.$$

PROOF. Take an (arbitrary) ε_1 obeying the conditions

$$(A.19a) \quad 0 < \varepsilon_1 \leq \frac{\sin \varepsilon}{8\pi}, \quad \varepsilon_1 < \left(\frac{1}{4\pi\varepsilon} - \tau_* \varkappa_{0,2} \right) \frac{\sin^2 \varepsilon}{4}.$$

REMARK. The second inequality on ε_1 is not necessary for the proof of the lemma. We included it here in order to define the radius R that will be admissible simultaneously here and in the main Lemma A.7 below. The constants τ_* and $\varkappa_{0,2}$ are defined in Remark A.6.

For ε_1 so chosen, let $R_1(\varepsilon_1)$ be the corresponding radius that Lemma A.3 gives. Denote by $R_{\mathfrak{T}}$ the following constant:

$$(A.19b) \quad R_{\mathfrak{T}} := \sup_{\substack{0 \leq t \leq T \\ |y|^2 + |\eta|^2 \leq r_{1/3}^2}} (|q(t, y, \eta)|^2 + |p(t, y, \eta)|^2)^{1/2},$$

where $r_{1/3}$ is the r_δ from Lemma A.2, corresponding to $\delta = 1/3$.

Define

$$(A.19c) \quad R = R(\varepsilon_1) = \max\{R_1(\varepsilon_1), r_{1/3}, R_{\mathfrak{T}}\}.$$

The conservation of energy ($H(q, p) = H(y, \eta)$) and inequalities (iii) of Lemma A.2 with $\delta = 1/3$ yield the estimates

$$(A.19d) \quad \sup_{|y|^2 + |\eta|^2 \leq R^2(\varepsilon_1)} |q(t, y, \eta)| \leq \sqrt{2}R(\varepsilon_1),$$

$$(A.19e) \quad M = \sup_{|y|^2 + |\eta|^2 = R^2(\varepsilon_1)} |q(t, y, \eta) - \cos t \cdot y - \sin t \cdot \eta| \leq 3R(\varepsilon_1).$$

The estimates (A.12) and Lemma A.3 then imply (a), (b), and (d).

Finally, to show that for every $(y, x) \in B_{\geq \varrho}$ there is a unique $(y, \eta) \in \mathbb{R}^{2n}$ such that $F_t(y, \eta) = (y, x)$, we notice that, if the equation $F_t(y, \eta) = (y, x)$ had a solution (y, η) in the ball $B_{< R}$, then we would have $|x|^2 \geq |y|^2 - |\eta|^2 = |x|^2 + |y|^2 - (|y|^2 + |\eta|^2) > \varrho^2 - R^2 > 16R^2$, which contradicts (A.19d). Hence, all the solutions to $F_t(y, \eta) = (y, x)$ must lie in $B_{\geq R}$, but there the solution is unique, as we have already proved in (a). The smoothness of F_t^{-1} follows from the inverse function theorem. \square

From now on, we assume that R is the number defined by (A.19c) with the help of an ε_1 satisfying (A.19a).

We are now in a position to define the action function $S(t, x, y)$ for y and x fulfilling the condition $|y|^2 + |x|^2 \geq \varrho^2$ with any of the ϱ 's provided by Lemma A.5. As usual,

$$(A.20) \quad S(t, x, y) = \int_0^t \left(\frac{1}{2} \left| \frac{\partial q(s, y, \eta)}{\partial s} \right|^2 - \frac{1}{2} |q(s, y, \eta)|^2 - w(q(s, y, \eta)) \right) ds,$$

where η is uniquely determined by the equation $F_t(y, \eta) = (y, x)$.

REMARK A.6. Recall that there exists $\tau_* > 0$ such that for $0 < t \leq \tau_*$ the action $S(t, x, y)$ is well defined for all $x, y \in \mathbb{R}^n$. The function $S(t, x, y)$ is smooth and, in addition,

$$(A.21) \quad S(t, x, y) = \frac{|x - y|^2}{2t} + t\Phi(t, x, y),$$

where $\Phi(t, x, y)$ satisfies the estimates

$$(A.22) \quad |\partial_x^\alpha \partial_y^\beta \Phi(t, x, y)| \leq \varkappa_{\alpha, \beta}, \quad \forall \alpha, \beta, \quad |\alpha + \beta| \geq 2,$$

with constants $\varkappa_{\alpha, \beta}$ independent of $t \in (0, \tau_*]$ and x, y . These facts are proved in [Fujiwara, 1979].

As mentioned at the beginning of this section, ε is chosen so that

$$(A.23a) \quad \frac{\tan \varepsilon}{\varepsilon} < \frac{4}{3}$$

and

$$(A.23b) \quad 0 < \varepsilon < \min \left\{ \frac{\tau_*}{4}, \frac{1}{4\pi\tau_*\varkappa_{0,2}} \right\}.$$

We list below the additional properties of $S(t, x, y)$ that we used in the main body of the paper.

LEMMA A.7.

- (a) $S(t, x, y)$ is a smooth function on $\mathfrak{T} \times B_{\geq \varrho}$.
- (b) Assume that s and θ are such that $0 < s < \tau_*$, $\theta \in \mathfrak{T}$, $s + \theta \in \mathfrak{T}$, and

$$(A.24) \quad \left| \cot \theta + \frac{1}{s} \right| \geq \frac{1}{4\varepsilon}.$$

Then, for all $x, y \in \mathbb{R}^n$, there exists a constant $\tilde{R} = \tilde{R}(x, y, s, \theta) > 0$ such that

$$(A.25) \quad \left| \frac{\partial}{\partial z} [S(s, x, z) + S(\theta, z, y)] \right| \geq \frac{1}{8\varepsilon} |z| \quad \text{when } |z| \geq \tilde{R}.$$

- (c) Let s and θ be as in part (b). Then

$$(A.26a) \quad \frac{\partial^2}{\partial z^2} [S(s, x, z) + S(\theta, z, y)] = \left(\cot \theta + \frac{1}{s} \right) \cdot \mathbf{1} + \Psi(s, \theta, x, y, z),$$

where Ψ is an $n \times n$ matrix with the following estimate on its norm:

$$(A.26b) \quad \|\Psi(s, \theta, x, y, z)\| \leq \frac{1}{\pi} \left| \cot \theta + \frac{1}{s} \right|$$

for all z such that $|z| \geq \varrho$, where ϱ is related to R by (A.17), and R is defined by (A.19c).

(d) Let s and θ be as in part (b). Define

$$\varrho_1 = 432(1 + 2\sqrt{2}\pi)(\sin \varepsilon)^{-2}\varrho.$$

Given x and y with $|x|^2 + |y|^2 \geq \varrho_1^2$, there exists a unique z_* (stationary point) such that

$$(A.27a) \quad \left. \frac{\partial}{\partial z} [S(s, x, z) + S(\theta, z, y)] \right|_{z=z_*} = 0,$$

and $|y|^2 + |z_*|^2 \geq \varrho^2$. This stationary point z_* is nothing but the point $q(\theta, y, \eta)$ on the trajectory connecting y and x in time $s + \theta$, and

$$(A.27b) \quad S(s, x, z_*) + S(\theta, z_*, y) = S(s + \theta, x, y).$$

(e) Under the assumptions of part (d),

$$(A.28) \quad \left| \frac{\partial}{\partial z} [S(s, x, z) + S(\theta, z, y)] \right| \geq \frac{1}{8\varepsilon} |z - z_*|.$$

(f) Under the assumptions of part (d), if $|z| \geq \varrho$, then

$$(A.29) \quad \left| \det \frac{\partial^2}{\partial z^2} [S(s, x, z) + S(\theta, z, y)] \right| \geq \left(\frac{4\pi\varepsilon}{\pi - 1} \right)^{-n}.$$

(g) Under the assumptions of part (d), all the derivatives of $S(s, x, z) + S(\theta, z, y)$ of order two and higher with respect to x , y , and z , are bounded:

$$(A.30) \quad \left| \left(\frac{\partial}{\partial x} \right)^\alpha \left(\frac{\partial}{\partial y} \right)^\beta \left(\frac{\partial}{\partial z} \right)^\sigma [S(s, x, z) + S(\theta, z, y)] \right| \leq C_{\alpha, \beta, \sigma}, \quad |\alpha| + |\beta| + |\sigma| \geq 2.$$

PROOF. Part (a) is obvious: use (A.20), Lemma A.5, and the inverse function theorem. We postpone the proof of (b) and turn to the proof of (c). Note that

$$(A.31a) \quad \left. \frac{\partial}{\partial z} S(\theta, z, y) \right|_{z=q(\theta, y, \eta)} = p(\theta, y, \eta),$$

and

$$(A.31b) \quad \left. \frac{\partial^2}{\partial z^2} S(\theta, z, y) \right|_{z=q(\theta, y, \eta)} = \frac{\partial}{\partial \eta} p(\theta, y, \eta) \cdot \left(\frac{\partial}{\partial \eta} q(\theta, y, \eta) \right)^{-1}.$$

By assumption, $|y|^2 + |z|^2 \geq \varrho^2$, and Lemma A.5 guarantees the uniqueness of η such that $q(\theta, y, \eta) = z$. From Lemma A.3, it follows that

$$(A.32a) \quad \frac{\partial}{\partial \eta} q(\theta, y, \eta) = \sin t \cdot \mathbf{1} + \vartheta_q(\theta, y, \eta),$$

$$(A.32b) \quad \frac{\partial}{\partial \eta} p(\theta, y, \eta) = \cos t \cdot \mathbf{1} + \vartheta_p(\theta, y, \eta),$$

where

$$(A.32c) \quad \|\vartheta_q(\theta, y, \eta)\| \leq \varepsilon_1, \quad \|\vartheta_p(\theta, y, \eta)\| \leq \varepsilon_1.$$

Since, by assumption, $\varepsilon_1 < \sin \varepsilon$ and $t \in \mathfrak{T}$, the matrix $\partial q / \partial \eta$ is invertible. We have

$$\begin{aligned} & (\cos t \cdot \mathbf{1} + \vartheta_p(\theta, y, \eta)) \cdot (\sin t \cdot \mathbf{1} + \vartheta_q(\theta, y, \eta))^{-1} - \cot t \cdot \mathbf{1} \\ &= \cot t \cdot \left(\mathbf{1} + \frac{1}{\sin t} \vartheta_q \right)^{-1} + \frac{1}{\sin t} \vartheta_p \cdot \left(\mathbf{1} + \frac{1}{\sin t} \vartheta_q \right)^{-1} - \cot t \cdot \mathbf{1} \\ &= \cot t \cdot \left(\mathbf{1} - \frac{1}{\sin t} \vartheta_q \left(\mathbf{1} + \frac{1}{\sin t} \vartheta_q \right)^{-1} \right) + \frac{1}{\sin t} \vartheta_p \cdot \left(\mathbf{1} + \frac{1}{\sin t} \vartheta_q \right)^{-1} - \cot t \cdot \mathbf{1} \\ &= \left(\frac{1}{\sin t} \vartheta_p - \frac{\cos t}{\sin^2 t} \vartheta_q \right) \cdot \left(\mathbf{1} + \frac{1}{\sin t} \vartheta_q \right)^{-1}. \end{aligned}$$

The norm of this matrix, for $t \in \mathfrak{T}$, is bounded by

$$\varepsilon_1 \cdot \frac{|\sin t| + |\cos t|}{\sin^2 t} \cdot \frac{1}{1 - \varepsilon_1 / \sin \varepsilon} \leq \frac{4\varepsilon_1}{\sin^2 \varepsilon},$$

because of (A.19a). Now, using the representation (A.21), (A.31b), (A.22) and the above estimate, we obtain

$$\frac{\partial^2}{\partial z^2} [S(s, x, z) + S(\theta, z, y)] - \left(\cot \theta + \frac{1}{s} \right) \cdot \mathbf{1} = \Psi(s, \theta, x, y, z),$$

where the right hand side has the norm bounded by

$$\frac{4\varepsilon_1}{\sin^2 \varepsilon} + s \mathfrak{A}_{0,2} \stackrel{(A.19a)}{\leq} \frac{1}{4\pi\varepsilon} \stackrel{(A.24)}{\leq} \frac{1}{\pi} \left| \cot \theta + \frac{1}{s} \right|,$$

and part (c) is proved. Part (b) follows from (c) and Lemma A.4 applied to $F(z) = \partial[S(s, x, z) + S(\theta, z, y)] / \partial z$.

To prove (d), we notice that if $|x|^2 + |y|^2 \geq \varrho_1^2$, then, by Lemma A.5, there exists a unique η such that $x = q(s + \theta, y, \eta)$. We also know that $|\eta|^2 + |y|^2 \geq R_1^2$, where R_1 is related to ϱ_1 by (A.17). Taking into account the relation between ϱ_1 and ϱ , we see that

$$(|\eta|^2 + |y|^2) \frac{\sin^2 \varepsilon}{16} \geq R_1^2 \frac{\sin^2 \varepsilon}{16} = \varrho^2.$$

On the other hand,

$$|y|^2 + |q(\theta, y, \eta)|^2 = |F_\theta(y, \eta)|^2 \underset{(A.18)}{\geq} (|\eta|^2 + |y|^2) \frac{\sin^2 \varepsilon}{16},$$

and we conclude that $|y|^2 + |q(\theta, y, \eta)|^2 \geq \varrho^2$. Set $z_* = q(\theta, y, \eta)$. Then (A.27b) holds, and (A.27a) holds as well, since $\partial S(s, x, z_*)/\partial z = -p(\theta, y, \eta)$ and $\partial S(s, z_*, y)/\partial z = +p(\theta, y, \eta)$. To show that z_* is the unique solution to (A.27a) with the property $|y|^2 + |z_*|^2 \geq \varrho^2$, we assume that there exists another solution, say, z' , and

$$(A.33) \quad |y|^2 + |z'|^2 \geq \varrho^2.$$

By (A.33), there is a unique Hamiltonian trajectory $q(t, y, \eta')$ connecting $y = q(0, y, \eta')$ with $z' = q(\theta, y, \eta')$ (Lemma A.5(c)). We also know that

$$\frac{\partial}{\partial z} S(\theta, z', y) = p(\theta, y, \eta').$$

On the other hand, since s is small, there is a unique Hamiltonian trajectory $q(t, z', \xi)$ connecting $z' = q(0, z', \xi)$ with $x = q(s, z', \xi)$ (Remark A.6), and

$$\frac{\partial}{\partial z} S(s, x, z') = -p(0, z', \xi) = -\xi.$$

If z' is a solution of (A.27a), then we must have $p(\theta, y, \eta') = \xi$, and, hence, two trajectories, from y to z' , and from z' to x , are two pieces of one Hamiltonian trajectory $q(t, y, \eta')$ connecting y with x in time $s + \theta$. However, since $|x|^2 + |y|^2 \geq \varrho_1^2 > \varrho^2$, such a trajectory is unique by Lemma A.5(c). Thus, $\eta' = \eta$ and, consequently, $z' = z_*$.

The estimate (A.28) follows from (d) and Lemma A.4(iv) applied to $F(z) = \partial[S(s, x, z) + S(\theta, z, y)]/\partial z$.

The estimate (A.29) is a simple corollary of (A.26) and (A.24). Indeed, for each vector $\xi \in \mathbb{R}^n$, we have

$$\left| \frac{\partial^2}{\partial z^2} [S(s, x, z) + S(\theta, z, y)] \xi \right| \underset{(A.26)}{\geq} \left(1 - \frac{1}{\pi} \right) \left| \cot \theta + \frac{1}{s} \right| |\xi| \underset{(A.24)}{\geq} \frac{\pi - 1}{4\pi\varepsilon} |\xi|,$$

and (A.29) follows.

To prove (A.30), one can estimate separately the derivatives of $S(s, x, z)$ and $S(\theta, z, y)$. The boundedness of the high-order derivatives of $S(s, x, z)$ with small s is a consequence of Fujiwara's result. The estimates on the derivatives of $S(\theta, z, y)$ can be obtained in the spirit of the proof of part (b). But we rather skip the proof not willing to bore the reader with more of lengthy and repetitious argument. \square

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