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Semiclassical scattering by the Coulomb potential

by

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ABSTRACT. – We consider quantum evolution generated by a hamiltonian $-\frac{\hbar^2}{2}\Delta + V$, where V is a Coulomb potential. For a certain class of wavefunctions with a Gaussian probability density we construct an approximate semiclassical time evolution. We show that the modified wave operators can be approximated in the leading order in $\hbar$ using the corresponding classical Møller transformations. © Elsevier, Paris

RÉSUMÉ. – Nous examinerons l'évolution quantique générée par l'hamiltonien $-\frac{\hbar^2}{2}\Delta + V$, où V est un potentiel de Coulomb. Pour une certaine classe de fonctions d'ondes avec une densité de probabilité gaussienne, nous construirons une solution approximative semi-classique dépendante du temps. Nous montrerons ainsi que les opérateurs d'ondes modifés peuvent être approchés à l'ordre dominant en $\hbar$ grâce à l'utilisation des transformations classiques de Møller correspondantes. © Elsevier, Paris

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1. INTRODUCTION

In quantum mechanical scattering theory one distinguishes two classes of potentials: short and long range. While for short range potentials the theory is fairly straightforward, in the long range case it can sometimes cause considerable difficulties. It has been long known that in this case the standard wave operators do not exist and the definitions need to be modified. The first such construction was given by Dollard [4] for the Coulomb potential. Since then several other approaches have been developed [2,17,11].

Classical scattering has been, rather surprisingly, a subject to much fewer papers than its quantum counterpart. One might mention here [16] for short and [9] for long rang problems, or a review of current results by Dereziński and Gerard [3]. In the classical case we see similar problems with the long range potentials and a suitably chosen free dynamics needs to be used.

In the present paper we consider the semiclassical approximation to the quantum scattering of a particle by the Coulomb potential. The idea is a generalization of the technique developed in [6,15] for the short range potentials. This approach is based on a certain Gaussian wavefunctions [6] called the semiclassical wavepackets. The quantum evolution of such wavepackets can be approximated in the leading order in $\hbar$ by a similar Gaussian "following" the classical trajectory of a particle with an appropriate phase change and spreading. It is interesting to note that such approximation to the free quantum evolution is in fact exact [6]. The result can be extended to an arbitrary order in $\hbar$ if the approximating state is taken as a superposition of products of Gaussians with certain generalizations of Hermite polynomials [8]. Also more general states can be considered [15].

For systems with Coulomb, or in general, long range interaction this technique encounters several difficulties. As already mentioned, in order to ensure the existence of the wave operators in both the quantum and classical case one needs to modify the free dynamics. This affects the semiclassical limit and a suitable modification is defined in this work. Even more important, it seems that under the long-range forces the propagation of a Gaussian state cannot be well approximated by merely scaling and translating it. Nevertheless we show that the error (albeit growing in time) is of the order $O(\hbar^{\frac{1}{2}})$. Consequently we construct an approximation to the Dollard wave operator.

The semiclassical approximation is a problem of its own, but our interest in it stems from the fact that it is a part of a rigorous treatment of the Born–Oppenheimer approximation [7]. The Born–Oppenheimer scattering for short range potentials is analyzed in [12,13], while the long range scattering is still an open problem.

The semiclassical scattering has been also studied by Yajima in the short [18] and long range case [19]. Yajima's approach is based on integral operator techniques developed by Hörmander [10] and Asada and Fujiwara [1,5]. The results are stronger than ours since he constructs an approximation to the wave operators and the scattering operator of order $O(\hbar)$. Yajima's technique is, however, restricted to the momentum representation, while our paper presents an approximation of order $o(1)$ to the wave operators in the position representation. We use only basic functional analysis tools and a quadratic approximation to the potential. Therefore we find our method not only much simpler, but also more intuitive, with the role of the classical trajectories much more apparent.

The rest of this paper is organized as follows. In Section 2 we explain the notation and state our main result, while the details of the proofs are given in Section 3.

2. NOTATION AND RESULTS

We consider the quantum dynamics generated by the hamiltonian of the form:

$$H(\hbar) = -\frac{\hbar^2}{2}\Delta + V \tag{1}$$

on $L^2(\mathbb{R}^n, dx)$, $n \geqslant 3$. Here $V(x) = \frac{1}{|x|}$ is the Coulomb potential. We also denote the free hamiltonian by:

$$H_0(\hbar) = -\frac{\hbar^2}{2}\Delta. \tag{2}$$

In particular we are concerned with the time-evolution generated by the hamiltonian (1) of so-called semiclassical wavepackets introduced by Hagedorn [6]. The definition is the following:

DEFINITION 1. – *Let A and B be complex $n \times n$ matrices satisfying*:

$$\begin{aligned} &\text{a) } A \text{ and } B \text{ are invertible},\\ &\text{b) } BA^{-1} \text{ is symmetric},\\ &\text{c) } Re\, BA^{-1} = \tfrac{1}{2}[BA^{-1} + (BA^{-1})^*] \text{ is strictly positive definite},\\ &\text{d) } (Re\, BA^{-1})^{-1} = AA^*. \end{aligned} \tag{3}$$

Also let $a \in \mathbb{R}^n$, $\eta \in \mathbb{R}^n$, $\eta \neq 0$, $\hbar > 0$. We define the semiclassical wavepacket as:

$$\phi(A, B, \hbar, a, \eta, x) = \pi^{-\frac{n}{4}}\hbar^{-\frac{n}{4}}(\det A)^{-\frac{1}{2}} \times \exp\left(-\frac{\langle (x-a), BA^{-1}(x-a)\rangle}{2\hbar} + \mathrm{i}\frac{\langle \eta, x-a\rangle}{\hbar}\right). \tag{4}$$

Remark 2. – Let $\mathcal{F}_\hbar f$ (or $\hat{f}^\hbar$) denote the scaled Fourier transform of f, i.e.:

$$\hat{f}^\hbar(\xi) = (\mathcal{F}_\hbar f)(\xi) := (2\pi\hbar)^{-\frac{n}{2}} \int_{\mathbb{R}^n} \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\langle x,\xi\rangle} f(x)\, dx. \tag{5}$$

Then [6]

$$\big(\mathcal{F}_\hbar \phi(A, B, \hbar, a, \eta, \cdot)\big)(\xi) = \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\langle \eta, a\rangle} \phi(B, A, \hbar, \eta, -a, \xi). \tag{6}$$

Remark 3. – From (6) one can see that ϕ is concentrated near position a and momentum η with widths determined by matrices A and B, respectively.

The quantum propagator associated with the hamiltonian (1) is:

$$T^\hbar(t) f(x) = \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}H(\hbar)t} f(x). \tag{7}$$

As we mentioned the wave operators exist if we replace the free propagator (generated by the free hamiltonian (2)) by a suitably defined modified free evolution. For a state f with $\hat{f}^\hbar \in C_0^\infty(\mathbb{R}^n \setminus \{0\})$ we define it as follows:
there is $t_0 > 0$ such that for $|t| > t_0$:

$$T_D^\hbar(t) f(x) = \mathcal{F}_\hbar^{-1}\left(\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\frac{\xi^2 t}{2} - \frac{\mathrm{i}}{\hbar}X_\hbar(\xi,t)} \hat{f}^\hbar(\xi)\right)(x). \tag{8}$$

Here

$$X_\hbar(\xi,t)=\operatorname{sgn}(t)\frac{\log(4\xi^2|t|)}{|\xi|} \tag{9}$$

is called a modifier. In fact what matters is the value of the modifier on *supp* $\hat{f}^\hbar$. Assuming *supp* $\hat{f}^\hbar \in ann(0,c_1,c_2)$ and denoting by $\chi(c_1,c_2,\xi)$ the characteristic function of the annulus $ann(0,c_1,c_2)$, we can replace (8) by:

$$T^\hbar_{D,c_1,c_2}(t)f(x)=\mathcal{F}_\hbar^{-1}\left(e^{-\frac{i}{\hbar}\frac{\xi^2 t}{2}-\frac{i}{\hbar}X_\hbar(\xi,t)}\chi(c_1,c_2,\xi)\hat{f}^\hbar(\xi)\right)(x). \tag{10}$$

Eq. (10) can be used to define the modified free evolution for an arbitrary state, not necessarily compactly supported. In particular this applies to the semiclassical wave packets. It is easy to see that:

$$\begin{aligned}
&\int_{|\xi|<c_1}\left|e^{-\frac{i}{\hbar}\frac{\xi^2 t}{2}-\frac{i}{\hbar}X_\hbar(\xi,t)}\hat{\phi}^\hbar(A,B,\hbar,a,\eta,\xi)\right|^2 d\xi\\
&\quad=K_1\hbar^{-\frac{n}{2}}\int_{|\xi|<c_1}\left|e^{-\frac{\langle\xi-\eta,AB^{-1}(\xi-\eta)\rangle}{2\hbar}}\right|^2 d\xi\\
&\quad\leqslant K_2\hbar^{-\frac{n}{2}}\int_{|\xi|<c_1}d\xi\to 0
\end{aligned}$$

as $c_1\to 0$, uniformly in t. Similarly:

$$\int_{|\xi|>c_2}\left|e^{-\frac{i}{\hbar}\frac{\xi^2 t}{2}-\frac{i}{\hbar}X_\hbar(\xi,t)}\hat{\phi}^\hbar(A,B,\hbar,a,\eta,\xi)\right|^2 d\xi\to 0$$

as $c_2\to\infty$, uniformly in t. It follows that:

$$\lim_{c_1\to 0,\ c_2\to\infty} T^\hbar_{D,c_1,c_2}(t)\phi(A,B,\hbar,a,\eta,x)$$

exists uniformly in t. We denote the limit by

$$\begin{aligned}
&T^\hbar_D(t)\phi(A,B,\hbar,a,\eta,x)\\
&\quad=\mathcal{F}_\hbar^{-1}\left(e^{-\frac{i}{\hbar}\frac{\xi^2 t}{2}-\frac{i}{\hbar}X_\hbar(\xi,t)}\hat{\phi}^\hbar(A,B,\hbar,a,\eta,\xi)\right)(x),
\end{aligned} \tag{11}$$

always remembering that a limiting procedure of the above kind is understood.

The modified (Dollard) wave operators are defined as:

$$\Omega^{\mp} = s\text{-}\lim_{t \to \pm\infty} T^{\hbar}(-t) T_D^{\hbar}(t). \tag{12}$$

The existence is a standard result [14].

Now we proceed to define the semiclassical dynamics. Let A_-, B_- be $n \times n$ complex matrices satisfying (3) and a_-, $\eta_- \in \mathbb{R}^n$ such that $\eta_- \neq 0$. Let $a(t)$, $\eta(t)$, $A(t)$, $B(t)$, $S(t)$ be a solution to the system of coupled ODE's:

$$\begin{aligned}
\frac{da}{dt} &= \eta, \\
\frac{d\eta}{dt} &= -V^{(1)}(a), \\
\frac{dA}{dt} &= \mathrm{i}B, \\
\frac{dB}{dt} &= \mathrm{i}V^{(2)}(a)A, \\
\frac{dS}{dt} &= \frac{\eta^2}{2} - V(a)
\end{aligned} \tag{13}$$

(where $V^{(1)}$ denotes the gradient of V and $V^{(2)}$ is the Hessian matrix) satisfying asymptotic conditions:

$$\begin{aligned}
&\lim_{t \to -\infty} \left| a_- + \eta_- t + \frac{\eta_-}{|\eta_-|^3} \log\left(\frac{4\eta_-^2 |t|}{\mathrm{e}^2}\right) - a(t) \right| = 0, \\
&\lim_{t \to -\infty} |\eta_- - \eta(t)| = 0, \\
&\lim_{t \to -\infty} \| A_- + D_- + \mathrm{i}tB_- + F_- \log(4\eta_-^2 |t|) - A(t) \| = 0, \\
&\lim_{t \to -\infty} \| B_- - B(t) \| = 0, \\
&\lim_{t \to -\infty} \left| \frac{\eta_-^2 t}{2} + \frac{2}{|\eta_-|} \log\left(\frac{4\eta_-^2 |t|}{\mathrm{e}}\right) - S(t) \right| = 0,
\end{aligned} \tag{14}$$

where

$$\begin{aligned}
(D_-)_{kl} &= -\frac{2\mathrm{i}(B_-)_{kl}}{|\eta_-|^3} + \frac{8\mathrm{i}\sum_j (\eta_-)_k (\eta_-)_j (B_-)_{jl}}{|\eta_-|^5}, \\
(F_-)_{kl} &= \frac{\mathrm{i}(B_-)_{kl}}{|\eta_-|^3} - \frac{3\mathrm{i}\sum_j (\eta_-)_k (\eta_-)_j (B_-)_{jl}}{|\eta_-|^5}.
\end{aligned} \tag{15}$$

Remark 4. – The first two equations (13) are the Hamilton's equations for a classical particle with position $a(t)$ and momentum $\eta(t)$. It is well known that such a particle moving in a Coulomb force field reaches an asymptotic momentum, but the asymptotic time parametrization of its orbit differs from the free motion with constant momentum by a logarithmic factor (cf. (14)).

Remark 5. – $S(t)$ is the action along the classical trajectory.

The semiclassical interacting time evolution of the wavepackets (4) is then given by:

$$U(t)\phi\big(A(0), B(0), \hbar, a(0), \eta(0), x\big) \\ = \mathrm{e}^{\frac{\mathrm{i}S(t)}{\hbar}}\phi\big(A(t), B(t), \hbar, a(t), \eta(t), x\big). \tag{16}$$

The corresponding semiclassical modified free dynamics is:

$$U_D(t)\phi(A_-, B_-, \hbar, a_-, \eta_-, x) = \mathrm{e}^{\frac{\mathrm{i}}{\hbar}\left(\frac{\eta_-^2 t}{2}+\frac{2}{|\eta_-|}\log\left(\frac{4\eta_-^2|t|}{\mathrm{e}}\right)\right)} \\ \times\phi\Bigg(A_- + D_- + \mathrm{i}tB_- + F_-\log\left(4\eta_-^2|t|\right), B_-, \hbar, \tag{17} \\ \times a_- + \eta_- t + \frac{\eta_-}{|\eta_-|^3}\log\left(\frac{4\eta_-^2|t|}{\mathrm{e}^2}\right), \eta_-, x\Bigg)$$

for $|t| > 1/4\eta_-^2$.

Remark 6. – For $|t| < 1/4\eta_-^2$ or if one is interested in the approximation to quantum dynamics on a finite time interval only, the logarithmic terms in (17) should be dropped.

Now we can state our main result, which we prove in the following section.

THEOREM 7. – *Let Ω^+ be a quantum wave operator defined in* (12). *Given $\varepsilon > 0$*

$$\left\|\Omega^+\phi(A_-, B_-, \hbar, a_-, \eta_-, \cdot) - \phi\big(A(0), B(0), \hbar, a(0), \eta(0), \cdot\big)\right\| < \varepsilon \tag{18}$$

for $\hbar$ small enough.

Remark 8. – The statement of the theorem and estimates in the following section are concerned with the $t \to -\infty$ limit. The proofs for large positive times are analogous.

Remark 9. – Theorem 7 simply says that the action of the quantum wave operator on Gaussian states (4) can be approximated by a corresponding classical Møller transformation $(a_-, \eta_-) \to (a(0), \eta(0))$. For short-range potentials the error in (18) is of order $O(\hbar^{\frac{1}{2}})$ [6]. Moreover in this case the estimate is uniform in time in a sense that:

$$\sup_{t\in\mathbb{R}} \Big\| e^{-\frac{itH(\hbar)}{\hbar}} \Omega^+ \phi(A_-, B_-, \hbar, a_-, \eta_-, \cdot) \\ - e^{\frac{iS(t)}{\hbar}} \phi\big(A(t), B(t), \hbar, a(t), \eta(t), \cdot\big) \Big\| < C\hbar^{\frac{1}{2}}. \tag{19}$$

For the Coulomb potential the norm in (19) apparently diverges as $\log t$.

3. TECHNICALITIES

We split the proof into several lemmas. The basic idea is very straightforward: we replace Ω^+ by its finite time analog $\Omega_t = T^{\hbar}(-t)T_D^{\hbar}(t)$ and approximate the quantum interacting and free propagators by the corresponding semiclassical ones.

LEMMA 10. – *Given A_-, B_-, a_-, η_- as described above, there is a solution to the system of ODE's* (13) *satisfying* (14). *In fact*:

$$\begin{aligned} a(t) &= a_- + \eta_- t + \frac{\eta_-}{|\eta_-|^3} \log\left(\frac{4\eta_-^2 |t|}{e^2}\right) + O\left(\frac{\log(|t|)}{|t|}\right), \\ \eta(t) &= \eta_- + O\left(\frac{1}{|t|}\right), \\ A(t) &= A_- + D_- + itB_- + F_- \log(4\eta_-^2 |t|) + O\left(\frac{\log(|t|)}{|t|}\right), \\ B(t) &= B_- + O\left(\frac{1}{|t|}\right). \end{aligned} \tag{20}$$

Proof. – We denote:

$$\begin{aligned} a_-(t) &= a_- + \eta_- t + \frac{\eta_-}{|\eta_-|^3} \log\left(\frac{4\eta_-^2 |t|}{e^2}\right), \\ \eta_-(t) &= \eta_-, \\ A_-(t) &= A_- + D_- + itB_- + F_- \log(4\eta_-^2 |t|), \\ B_-(t) &= B_-, \\ S_-(t) &= \frac{\eta_-^2 t}{2} + \frac{2}{|\eta_-|} \log\left(\frac{4\eta_-^2 |t|}{e}\right). \end{aligned} \tag{21}$$

Consider a Banach space C_T of bounded, continuous functions y such that:

$$\|y\|_{C_T} := \left\| \frac{|t|}{\log(|t|)} y \right\|_{\infty,T} < \infty,$$

where $\|\cdot\|_{\infty,T}$ means a supremum over the interval $(-\infty, T)$. Let

$$\varphi(y(t)) := \int_{-\infty}^{t} d\tau \int_{-\infty}^{\tau} d\theta \left[V^{(1)}(\eta_{-}\theta) - V^{(1)}\left(a_{-}(\theta) + y(\theta)\right)\right], \tag{22}$$

then

$$\left|\varphi(y(t))\right| \leqslant \int_{-\infty}^{t} d\tau \int_{-\infty}^{\tau} d\theta \left| \frac{\eta_{-}}{|\eta_{-}|^3} \log\left(\frac{4\eta_{-}^2|\theta|}{\mathrm{e}^2}\right) + a_{-} + y(\theta) \right| \frac{C}{|\eta_{-}\theta|^3}.$$

If $\|y\|_{C_T} < \infty$, then

$$\left\|\varphi(y(t))\right\|_{C_T} := \left\| \frac{|t|}{\log(|t|)} \varphi(y(t)) \right\|_{\infty,T} < \infty,$$

i.e., φ maps C_T onto itself. Similarly for $y_1, y_2 \in C_T$:

$$\begin{aligned}
&\left|\varphi(y_1) - \varphi(y_2)\right| \\
&\quad \leqslant \left| \int_{-\infty}^{t} d\tau \int_{-\infty}^{\tau} d\theta \left[V^{(1)}\left(a_{-}(\theta) + y_1(\theta)\right) - V^{(1)}\left(a_{-}(\theta) + y_2(\theta)\right)\right] \right| \\
&\quad \leqslant \int_{-\infty}^{t} d\tau \int_{-\infty}^{\tau} d\theta C \left| y_1(\theta) - y_2(\theta) \right| \frac{\log(|\theta|)}{|\eta_{-}\theta|^3}.
\end{aligned}$$

Hence

$$\begin{aligned}
\left\|\varphi(y_1) - \varphi(y_2)\right\|_{C_T} &\leqslant \sup_{t<T} \frac{|t|}{\log(|t|)} \left|\varphi(y_1) - \varphi(y_2)\right| \\
&\leqslant \sup_{t<T} \left[\frac{|t|}{\log(|t|)} \sup_{s<t} \left(\left|\varphi(y_1) - \varphi(y_2)\right| \frac{|s|}{\log(|s|)} \right) \right. \\
&\qquad \left. \times \int_{-\infty}^{t} d\tau \int_{-\infty}^{\tau} d\theta C \frac{\log(|\theta|)^2}{|\theta|^4} \right] \\
&\leqslant \|y_1 - y_2\|_{C_T} \sup_{t<T} \left[\frac{|t|}{\log(|t|)} \int_{-\infty}^{t} d\tau \int_{-\infty}^{\tau} d\theta C \frac{\log(|\theta|)^2}{|\theta|^4} \right],
\end{aligned}$$

i.e., φ is a strict contraction for T sufficiently negative. By the contraction mapping principle the equation:

$$y(t) = \varphi\big(y(t)\big)$$

has a unique solution, which we denote by $u(t)$. One can immediately see that $a(t) = a_-(t) + u(t)$ solves the equation

$$\frac{d^2a}{dt^2} = -V^{(1)}(a),$$

and

$$u(t) = \mathrm{O}\left(\frac{\log(|t|)}{|t|}\right)$$

as $t \to -\infty$. Moreover:

$$|\eta(t) - \eta_-| = \left|\frac{\eta_-}{|\eta_- t|^3} + \dot{u}(t)\right| = \mathrm{O}\left(\frac{1}{|t|}\right).$$

Next we want to show:

$$A(t) = A_-(t) + \mathrm{O}\left(\frac{\log(|t|)}{|t|}\right),$$

$$B(t) = B_-(t) + \mathrm{O}\left(\frac{1}{|t|}\right).$$

Let Y_T be a space of matrix valued functions Z such that:

$$\|Z\|_{Y_T} := \sup_{t<T}\left\|\frac{|t|}{\log(|t|)}Z(t)\right\| < \infty,$$

where $\|M\|$ is the Euclidean norm of matrix M. We consider the mapping:

$$\mathcal{G}(Z(t)) := \int_{-\infty}^{t} d\tau \int_{-\infty}^{\tau} d\theta \left[-V^{(2)}(a(\theta))(A_-(\theta) + Z(\theta)) + \frac{G\theta}{|\eta_-|^3\theta^3}\right], \tag{23}$$

where

$$(G)_{kl} = \mathrm{i}(B_-)_{kl} - \frac{3\mathrm{i}}{|\eta_-|^2}\sum_j (\eta_-)_k(\eta_-)_j(B_-)_{jl}.$$

Using assumptions on the potential and asymptotics of $a(t)$ that we just proved, we show:

$$\|\mathcal{G}(Z(t))\|_{Y_T} = \sup_{t<T} \frac{|t|}{\log(|t|)} \|\mathcal{G}(Z(t))\|$$

and

$$\|\mathcal{G}(Z(t))\| \leqslant \int_{-\infty}^{t} d\tau \int_{-\infty}^{\tau} d\theta \mathcal{I}(\theta, Z(\theta)).$$

The integrand satisfies

$$\mathcal{I}(\theta, Z(\theta)) \leqslant \|V^{(2)}(a(\theta)) - V^{(2)}(\eta_- \theta)\| \|A_-(\theta) + Z(\theta)\| + \|W(\theta, Z(\theta))\|,$$

where W denotes a matrix with entries:

$$W_{kl} = \sum_j \left[\frac{\delta_{kj}}{|\eta_-|^3 \theta^3} - \frac{3(\eta_-)_k (\eta_-)_j \theta^2}{|\eta_-|^5 \theta^5} \right] \left(A_-(\theta) + Z(\theta) - \mathrm{i} B_- \theta\right)_{jl}.$$

Then

$$\mathcal{I}(\theta, Z(\theta)) \leqslant \frac{C \log(|\theta|)}{|\theta|^4} \|A_-(\theta) + Z(\theta)\| + \frac{C}{|\theta|^3} \|A_-(\theta) + Z(\theta) - \mathrm{i} B_- \theta\|.$$

This shows that $\mathcal{G}$ maps Y_T onto itself. Similar estimates show that:

$$\|\mathcal{G}(Z_1) - \mathcal{G}(Z_2)\|_{Y_T} \leqslant \|Z_1 - Z_2\|_{Y_T} \sup_{t<T} \frac{|t|^\alpha}{\log(|t|)} \int_{-\infty}^{t} d\tau \int_{-\infty}^{\tau} d\theta \|V^{(2)}(a(\theta))\| \frac{\log(|\theta|)}{|\theta|}$$

for any $0 < \alpha < 1$. Therefore for T sufficiently negative $\mathcal{G}$ is a strict contraction. As before, by the contraction mapping theorem the equation $Z = \mathcal{G} Z$ has a unique solution $U(t)$. One can easily verify that

$$A(t) = A_-(t) + U(t)$$

satisfies

$$\frac{d^2 A}{dt^2} = -V^{(2)}(a(t)) A(t),$$

and

$$\|B(t) - B_-\| = \left\| \frac{F_-}{t} + \dot{U}(t) \right\| = \mathrm{O}\left(\frac{1}{|t|}\right).$$

Finally we consider the phase. Let:

$$K(t) = \int_{-\infty}^{t} \left[\frac{\eta(\tau)^2}{2} - V\big(a(\tau)\big) - \frac{\eta_-^2}{2} + 2V(\eta_-\tau) \right] d\tau.$$

By the energy conservation $\frac{\eta_-^2}{2} = \frac{\eta(t)^2}{2} + V(a(t))$ for any t, so that:

$$|K(t)| = \left| 2 \int_{-\infty}^{t} d\tau \left[V\big(a(\tau)\big) - V(\eta_-\tau) \right] \right| \leqslant C \frac{\log(|t|)}{|t|}.$$

Then $|S(t) - S_-(t)| = |K(t)| \to 0$ as $t \to -\infty$. □

LEMMA 11. –

$$\begin{aligned} &\mathcal{F}_\hbar\big(U_D(t)\phi(A_-, B_-, \hbar, a_-, \eta_-, \cdot)\big)(\xi) \\ &\quad = \exp\left(-\frac{\mathrm{i}t\xi^2}{2\hbar}\right) \exp\left[\frac{\mathrm{i}}{\hbar} \left[\frac{\log(4\eta_-^2|t|)}{|\eta_-|} - \frac{\langle \xi - \eta_-, \eta_- \rangle}{|\eta_-|^3} \right.\right. \\ &\qquad \times \log\left(\frac{4\eta_-^2|t|}{\mathrm{e}^2}\right) - \frac{\langle \xi - \eta_-, \xi - \eta_- \rangle}{2|\eta_-|^3} \\ &\qquad \times \log\left(\frac{4\eta_-^2|t|}{\mathrm{e}^2}\right) - \frac{\langle \xi - \eta_-, \eta_- \rangle^2}{2|\eta_-|^5} \\ &\qquad \left.\left. \times \big(8 - 3\log(4\eta_-^2|t|)\big) \right] \right] \hat{\phi}^\hbar(A_-, B_-, \hbar, a_-, \eta_-, \xi). \end{aligned} \tag{24}$$

Proof. – By explicit calculations using (6) and (17). □

We use Lemma 11 to prove:

LEMMA 12. –

$$\begin{aligned} &\big\| \mathcal{F}_\hbar\big[T_D^\hbar(t)\phi(A_-, B_-, \hbar, a_-, \eta_-, x)\big](\cdot) \\ &\quad - \mathcal{F}_\hbar\big[U_D(t)\phi(A_-, B_-, \hbar, a_-, \eta_-, x)\big](\cdot) \big\| \leqslant C \log(|t|)\hbar^\lambda \end{aligned} \tag{25}$$

for any $\lambda \in (0, 1/2)$ *and* t *sufficiently negative.*

Proof. – Clearly it is enough to show:

$$\begin{aligned}&\left\|\mathcal{F}_\hbar\left[T^\hbar_{D,c_1,c_2}(t)\phi(A_-,B_-,\hbar,a_-,\eta_-,x)\right](\cdot)\right.\\&\quad\left.-\mathcal{F}_\hbar\left[U_D(t)\phi(A_-,B_-,\hbar,a_-,\eta_-,x)\right](\cdot)\chi(c_1,c_2,\cdot)\right\|\\&\quad\leqslant C\log(|t|)\hbar^\lambda\end{aligned}\tag{26}$$

with the constant C independent of c_1 and c_2. The left hand side of (26) equals:

$$\begin{aligned}&\left\|\exp\left(-\frac{it\xi^2}{2\hbar}+\frac{\mathrm{i}\log(4\xi^2|t|)}{\hbar|\xi|}\right)\chi(c_1,c_2,\xi)\hat{\phi}^\hbar(A_-,B_-,\hbar,a_-,\eta_-,\xi)\right.\\&\quad-\exp\left(-\frac{it\xi^2}{2\hbar}\right)\exp\left[\frac{i}{\hbar}\left[\frac{\log(4\eta_-^2|t|)}{|\eta_-|}-\frac{\langle\xi-\eta_-,\eta_-\rangle}{|\eta_-|^3}\log\left(\frac{4\eta_-^2|t|}{\mathrm{e}^2}\right)\right.\right.\\&\quad-\frac{\langle\xi-\eta_-,\xi-\eta_-\rangle}{2|\eta_-|^3}\log\left(\frac{4\eta_-^2|t|}{\mathrm{e}^2}\right)\\&\quad\left.\left.-\frac{\langle\xi-\eta_-,\eta_-\rangle^2}{2|\eta_-|^5}\left(8-3\log(4\eta_-^2|t|)\right)\right]\right]\\&\quad\left.\times\chi(c_1,c_2,\xi)\hat{\phi}^\hbar(A_-,B_-,\hbar,a_-,\eta_-,\xi)\right\|\\&\leqslant\frac{1}{\hbar}\left\|\left|X_\hbar(\xi,t)-Y_\hbar(\xi,\eta_-,t)\right|\chi(c_1,c_2,\xi)\right.\\&\quad\left.\times\hat{\phi}^\hbar(A_-,B_-,\hbar,a_-,\eta_-,\xi)\right\|\end{aligned}\tag{27}$$

$Y_\hbar(\xi,\eta_-,t)$ denotes the second order Taylor expansion of $X_\hbar(\xi,t)$ around $\xi=\eta_-$. By standard estimates:

$$\begin{aligned}&\left|X_\hbar(\xi,t)-Y_\hbar(\xi,\eta_-,t)\right|\\&\quad\leqslant|\xi-\eta_-|^3\sup_{p\in[\xi,\eta_-]}\left(\frac{K_1}{|p|^4}+\frac{K_2|\log(4p^2|t|)|}{|p|^4}\right)\end{aligned}\tag{28}$$

for some constants K_1, K_2. Here $[\xi,\eta_-]$ is the line segment connecting ξ and η_-.

Let

$$B_1=\{\xi\colon\ |\xi-\eta_-|<\hbar^\alpha|\eta_-|\},\quad\alpha=\frac{1+\lambda}{3},$$

$$B_2 = \{\xi\colon\ |\xi| < \mu|\eta_-|\}, \quad 0 < \mu < 1,$$
$$B_3 = \{\xi\colon\ |\xi| \geqslant \mu|\eta_-|, |\xi - \eta_-| \geqslant \hbar^\alpha|\eta_-|\}, \tag{29}$$

and let χ_1, χ_2, χ_3 be the corresponding characteristic functions. Then $1 = \chi_1 + \chi_2 + \chi_3$ and we split (27) into a sum of three terms of the form

$$I_k = \frac{1}{\hbar}\Big\| |X_\hbar(\xi, t) - Y_\hbar(\xi, \eta_-, t)| \chi(c_1, c_2, \xi)\chi_k(\xi) \times \hat{\phi}^\hbar(A_-, B_-, \hbar, a_-, \eta_-, \xi)\Big\|. \tag{30}$$

Each term is estimated separately. On B_1 we use (28). By the triangle inequality

$$\sup_{p\in[\xi,\eta_-]} \frac{1}{|p|^4} \leqslant \left(|\eta_-| - |\xi - \eta_-|\right)^{-4}.$$

Also

$$0 \leqslant \sup_{p\in[\xi,\eta_-]} \left|\log\left(4p^2|t|\right)\right| \leqslant C\log(|t|)$$

for $t < \min(-1, \inf_{\xi\in B_1}(-1/4\xi^2))$. Hence:

$$\begin{aligned} I_1 &\leqslant C\frac{\log(|t|)}{\hbar}\Big\| |\xi - \eta_-|^3\left(|\eta_-| - |\xi - \eta_-|\right)^{-4}\chi_1(\xi) \\ &\quad \times \chi(c_1, c_2, \xi)\hat{\phi}^\hbar(A_-, B_-, \hbar, a_-, \eta_-, \xi)\Big\| \\ &\leqslant C\log(|t|)\hbar^{3\alpha-1}\|\hat{\phi}^\hbar(A_-, B_-, \hbar, a_-, \eta_-, \xi)\| \\ &\leqslant C\hbar^\lambda\log(|t|) \end{aligned} \tag{31}$$

with a constant depending only on $|\eta_-|$. Here and in the rest of this work C denotes a generic constant.

An estimate for I_2 uses explicit forms of $X_\hbar$ and $Y_\hbar$. Then

$$\begin{aligned} I_2 &\leqslant \frac{1}{\hbar}\left\| \frac{|\log(4\xi^2|t|)|}{|\xi|}\chi_2(\xi)\chi(c_1, c_2, \xi)\hat{\phi}^\hbar(A_-, B_-, \hbar, a_-, \eta_-, \xi)\right\| \\ &\quad + \frac{1}{\hbar}\Big\| |Y_\hbar(\xi, \eta_-, t)|\chi_2(\xi)\chi(c_1, c_2, \xi)\hat{\phi}^\hbar(A_-, B_-, \hbar, a_-, \eta_-, \xi)\Big\|. \end{aligned} \tag{32}$$

On the first term in (32) we use the Hölder's inequality:

$$\frac{1}{\hbar}\left\| \frac{|\log(4\xi^2|t|)|}{|\xi|}\chi_2(\xi)\chi(c_1, c_2, \xi)\hat{\phi}^\hbar(A_-, B_-, \hbar, a_-, \eta_-, \xi)\right\|$$

$$\leqslant \frac{1}{\hbar}\left\|\frac{|\log(4\xi^2|t|)|}{|\xi|}\chi_2(\xi)\right\|_{L^2} \times \left\|\chi_2(\xi)\chi(c_1, c_2, \xi)\hat{\phi}^{\hbar}(A_-, B_-, \hbar, a_-, \eta_-, \xi)\right\|_{L^\infty}. \tag{33}$$

The first factor in (33) can be computed explicitly:

$$\left\|\frac{|\log(4\xi^2|t|)|}{|\xi|}\chi_2(\xi)\right\|_{L^2} = \left(\int_{B_2}\frac{|\log(4\xi^2|t|)|^2}{|\xi|^2}d\xi\right)^{\frac{1}{2}} \leqslant C\log\left(|t|\right) \tag{34}$$

for some constant $C = C(\eta_-)$ and $|t|$ big enough ($|t| > \max(1, (4\eta_-^2\mu^2)^{-1})$). Also from (4)

$$\begin{aligned}\left\|\chi_2(\xi)\chi(c_1, c_2, \xi)\hat{\phi}^{\hbar}(A_-, B_-, \hbar, a_-, \eta_-, \xi)\right\|_{L^\infty} &\leqslant \left\|\chi_2(\xi)\hat{\phi}^{\hbar}(A_-, B_-, \hbar, a_-, \eta_-, \xi)\right\|_{L^\infty} \\ &\leqslant C\hbar^{-\frac{n}{4}}e^{-\frac{C'}{\hbar}}\end{aligned} \tag{35}$$

for constants C, C' depending on $|\eta_-|$, $\|B_-\|$ and μ. The estimate for the second term in (32) is now straightforward:

$$\begin{aligned}&\frac{1}{\hbar}\left\||Y_\hbar(\xi, \eta_-, t)|\chi_2(\xi)\chi(c_1, c_2, \xi)\hat{\phi}^{\hbar}(A_-, B_-, \hbar, a_-, \eta_-, \xi)\right\| \\ &\quad\leqslant \frac{1}{\hbar}C\log\left(|t|\right)\left\|\chi_2(\xi)\hat{\phi}^{\hbar}(A_-, B_-, \hbar, a_-, \eta_-, \xi)\right\| \\ &\quad\leqslant C\log\left(|t|\right)\hbar^{-\frac{n}{4}-1}e^{-\frac{C'}{\hbar}}\end{aligned} \tag{36}$$

for $C = C(\eta_-)$, $|t| > \max(1, (4\eta_-)^{-1})$. Combining (34), (35) and (37) we get:

$$I_2 \leqslant C\log\left(|t|\right)\hbar^m \tag{37}$$

for $|t|$ large enough, m arbitrary.

The remaining term I_3 can be written in a form analogous to (32). For the part involving $X_\hbar$, for instance, we have:

$$\begin{aligned}&\frac{1}{\hbar}\left\|\frac{|\log(4\xi^2|t|)|}{|\xi|}\chi_3(\xi)\chi(c_1, c_2, \xi)\hat{\phi}^{\hbar}(A_-, B_-, \hbar, a_-, \eta_-, \xi)\right\| \\ &\quad\leqslant \frac{1}{\hbar}\left\|\chi_3(\xi)\frac{|\log(4\xi^2|t|)|}{|\xi|}e^{-\frac{1}{4\hbar}|B_-^{-1}(\xi-\eta_-)|^2}\right\|_{L^\infty} \\ &\quad\quad\times\left\|\pi^{-\frac{n}{4}}\hbar^{-\frac{n}{4}}\left(\det(B_-)\right)^{-\frac{1}{2}}e^{-\frac{1}{4\hbar}|B_-^{-1}(\xi-\eta_-)|^2}\right\|_{L^2}.\end{aligned} \tag{38}$$

By assumption $4\eta_-^2|t| > 1$, so there is T depending on μ and $|\eta_-|$ such that $4\xi^2|t| > 1$ for $|t| > T$ and $\xi \in B_3$. Then (38) is bounded by:

$$\frac{1}{\hbar}C\log(|t|)\mathrm{e}^{-\frac{1}{4\hbar}\|B_-\|^{-2}\hbar^{2\alpha}|\eta_-|^2} \leqslant \frac{1}{\hbar}C\log(|t|)\mathrm{e}^{-\frac{C'}{\hbar^{\varepsilon}}},$$

where $\varepsilon = 1 - 2\alpha > 0$. We note that C again depends only on $|\eta_-|$. The estimate for the rest of I_3 is analogous. □

LEMMA 13. –

$$\begin{aligned}\Big\|T^{\hbar}(t)\phi\big(A(0), B(0), \hbar, a(0), \eta(0), \cdot\big) \\ - \mathrm{e}^{\frac{\mathrm{i}S(t)}{\hbar}}\phi\big(A(t), B(t), \hbar, a(t), \eta(t), \cdot\big)\Big\| \leqslant Cg(t)\hbar^{\lambda}\end{aligned} \tag{39}$$

for any $0 < \lambda < \frac{1}{2}$, *where*

$$\lim_{t\to-\infty}\frac{g(t)}{\log(|t|)} = \text{const.} \tag{40}$$

Proof. –

$$\begin{aligned}&\big\|T^{\hbar}(t)\phi\big(A(0), B(0), \hbar, a(0), \eta(0), \cdot\big) - \mathrm{e}^{\frac{\mathrm{i}S(t)}{\hbar}} \\ &\quad\times\phi\big(A(t), B(t), \hbar, a(t), \eta(t), \cdot\big)\big\| \\ &\quad\leqslant \big\|\phi\big(A(0), B(0), \hbar, a(0), \eta(0), \cdot\big) - T^{\hbar}(-t)\mathrm{e}^{\frac{\mathrm{i}S(t)}{\hbar}} \\ &\qquad\times\phi\big(A(t), B(t), \hbar, a(t), \eta(t), \cdot\big)\big\| \\ &\quad\leqslant \frac{1}{\hbar}\int_0^t \Big\|\Big(H(\hbar) - \mathrm{i}\hbar\frac{d}{ds}\Big)\mathrm{e}^{\frac{\mathrm{i}S(s)}{\hbar}}\phi\big(A(s), B(s), \hbar, a(s), \eta(s), \cdot\big)\Big\|\,ds \\ &\quad= \frac{1}{\hbar}\int_0^t \big\||V(\cdot) - W_{a(s)}(\cdot)|\phi\big(A(s), B(s), \hbar, a(s), \eta(s), \cdot\big)\big\|\,ds.\end{aligned} \tag{41}$$

The last equality follows from

$$\begin{aligned}&\mathrm{i}\hbar\frac{d}{ds}\Big(\mathrm{e}^{\frac{\mathrm{i}S(s)}{\hbar}}\phi\big(A(s), B(s), \hbar, a(s), \eta(s), x\big)\Big) \\ &\quad= \Big(-\frac{\hbar^2}{2}\Delta + W_{a(s)}(x)\Big)\Big(\mathrm{e}^{\frac{\mathrm{i}S(s)}{\hbar}}\phi\big(A(s), B(s), \hbar, a(s), \eta(s), x\big)\Big),\end{aligned}$$

where $W_{a(s)}$ is the second order Taylor expansion of the potential around $a(s)$. From (41) we see that if:

$$\left\| \left| V(\cdot) - W_{a(s)}(\cdot) \right| \phi\left(A(s), B(s), \hbar, a(s), \eta(s), \cdot\right) \right\| \leqslant f(s)\hbar^{1+\lambda} \qquad (42)$$

for f such that $g(t) = \int_0^t f(s)\,ds$ satisfies (40), then (39) follows. The proof of (42) is a slight modification of a proof of analogous result for short range potentials [6]. □

LEMMA 14. – *Given* $\varepsilon > 0$:

$$\left\| U_D(t)\phi_- - U(t)\phi(0) \right\| < \varepsilon \qquad (43)$$

for $|t|$ *sufficiently large and* $\hbar$ *sufficiently small.*

Proof. – After a change of variables from x to $x - a(t)$ the left hand side of (43) it becomes:

$$\left\| e^{\frac{iS_-(t)}{\hbar}} \phi\left(A_-(t), B_-(t), \hbar, u(t), \eta_-(t), \cdot\right) - e^{\frac{iS(t)}{\hbar}} \phi\left(A(t), B(t), \hbar, 0, \eta(t), \cdot\right) \right\|,$$

where $u(t) = a(t) - a_-(t)$ (cf. Proof of Lemma 10).

Now we choose $T \ll 0$ and consider sets:

$$B_1 = \{x\colon\ |x| < ct\},$$
$$B_2 = \{x\colon\ |x| > ct\}$$

for some constant c $(t < T)$. Let χ_1 and χ_2 denote the corresponding characteristic functions. Denoting:

$$f(x,t) = e^{\frac{iS_-(t)}{\hbar}} \phi\left(A_-(t), B_-(t), \hbar, u(t), \eta_-(t), \cdot\right) - e^{\frac{iS(t)}{\hbar}} \phi\left(A(t), B(t), \hbar, 0, \eta(t), \cdot\right)$$

we have:

$$\left\| f(x,t) \right\|_{L^2} = \left\| \chi_1(x) f(x,t) \right\| + \left\| \chi_2(x) f(x,t) \right\| = I_1 + I_2.$$

First term can be estimated as follows: expand $f(x,t)$ in Taylor series in parameters a, η, A, and B. It is easy to see (from Lemma 10) that $f(x,t) \to 0$ as $t \to -\infty$ pointwise in x. By the dominated convergence theorem $\|\chi_1(x) f(x,t)\| \to 0$ as $t \to -\infty$ and the convergence is uniform in $\hbar$. It remains to estimate I_2. We note that it is an integral over the "tails" of the Gaussian wavepacket. Using the Hölder inequality in a manner similar to (38) we show:

$$I_2 < C\mathrm{e}^{-\frac{C'}{\hbar}}. \quad \square$$

Proof of Theorem 7. – Denote:

$$\phi_- = \phi\big(A_-, B_-, \hbar, a_-, \eta_-, \cdot\big),$$
$$\phi(t) = \phi\big(A(t), B(t), \hbar, a(t), \eta(t), \cdot\big).$$

Then:

$$\|\Omega^+\phi_- - \phi(0)\| \leqslant \|\Omega^+\phi_- - T^\hbar(-t)T_D^\hbar(t)\phi_-\| + \|T^\hbar(-t)T_D^\hbar(t)\phi_- - \phi(0)\| \leqslant I_1 + I,$$

where I can be further decomposed into:

$$\begin{aligned} I &= \|T_D^\hbar(t)\phi_- - T^\hbar(t)\phi(0)\| \\ &\leqslant \|T_D^\hbar(t)\phi_- - U_D(t)\phi_-\| + \|U_D(t)\phi_- - U(t)\phi(0)\| \\ &\quad + \|U(t)\phi(0) - T^\hbar(t)\phi(0)\| \leqslant I_2 + I_3 + I_4. \end{aligned}$$

A standard existence proof for Ω^+ (see, e.g., [14]) Theorem IX.9 where we merely inserted $\hbar$ in appropriate places) shows that there is $T > 0$ such that for $t < -T$ $I_1 < \varepsilon/4$ uniformly in $\hbar$. From Lemma 14 $I_3 < \varepsilon$. We choose $t < -\hbar^{-\gamma}$ for some $\gamma > 1$. Then by Lemmas 12 and 13:

$$I_2 < C\log\big(|\hbar^{-\gamma}|\big)\hbar^\lambda,$$
$$I_4 < Cg\big(\hbar^{-\gamma}\big)\hbar^\lambda.$$

Choosing $\hbar$ sufficiently small we prove (18). $\square$

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