Semi-classical Propagation on $|\log \hbar|$-Time-Scales

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Abstract We study the quantum evolution of a coherent state originally located in phase space on the unstable fixed point of a multiple well potential in one dimension. We show that for sufficiently long times the coherent state "splits" into two distinct components, each of which localizes semi-classically on a neighbouring unstable fixed point. We show moreover that during the transition the coherent state is distributed along the classical trajectory joining the two unstable points according to a density which we compute explicitly. At the times we explore the quantum dynamics of the coherent state it is no longer determined by the classical dynamics of its center, but rather by the classical dynamics of the trajectories that are at a distance $\sqrt{\hbar}$ of its center.

1 Introduction

There has been a growing interest in the last few years in the rigorous study of quantum dynamical systems in the semi-classical limit ($\hbar \to 0$) for "long" times, meaning for times t going to infinity as $\hbar$ tends to 0 [DB] [CR] [BGP] [BR] [BDB1] [HJ] [BDB2]. If the classical dynamics is stable, such as in completely integrable systems, standard techniques of semi-classical analysis allow one to obtain control on the quantum dynamics in terms of (semi-)classical expressions up to times of order $\hbar^{-k}$, for some $k > 0$. In the presence of instabilities however (unstable fixed points or periodic orbits, for example), these estimates tend to break down on much shorter time scales that are only logarithmic in $\hbar$. A good understanding of the quantum dynamics on as long a time scale as possible is important in quantum chaos, and has attracted considerable attention in this context [BB] [CC] [OTH] [TH], but not much is known rigorously. In the case of certain chaotic quantum maps, it was shown in [DB] and [BDB1] [BDB2] that already on the relatively short logarithmic time scale, interesting phenomena occur.

Here we want to address this same question in the context of a one-dimensional Schrödinger equation, close to a hyperbolic fixed point of the dynamics. This is arguably the simplest exponential instability that can occur in a Hamiltonian system. More precisely, we consider the time dependent Schrödinger equation

$$i\hbar\frac{\partial\psi(t)}{\partial t} = (-\frac{\hbar^2}{2}\frac{d^2}{dq^2} + V)\psi(t), \quad \psi(t_0) = \eta_\varepsilon, \tag{1}$$

where $V(q)$ is a smooth real potential depending on the position variable $q \in \mathbb{R}$ and η_ε is the usual L^2-normalized Gaussian living at the origin $(0,0)$ of the phase space, depending on a small parameter ε,

$$\eta_\varepsilon(q) = (\varepsilon^2\pi)^{-1/4} \ \exp\left(-\frac{q^2}{2\varepsilon^2}\right). \tag{2}$$

We will suppose V is a multiple well potential with a local maximum (barrier top) at $q = 0$, leading to an unstable fixed point at $X_0 = (0,0)$ (Fig. 1). The Hamiltonian $\hat{H} := -\frac{\hbar^2}{2}\frac{d^2}{dq^2} + V$ is self-adjoint on a suitable domain in $L^2(\mathbb{R})$. The stationary

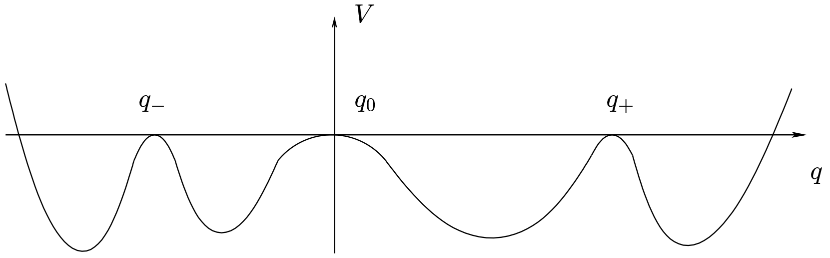

Figure 1: A confining quadruple well potential

problem close to the critical energy $E = 0$ was studied in this setting in much detail by Colin de Verdière and Parisse [CP1, CP2] and also by Toth [T]. Here we are interested in the time-dependent problem: more precisely, we wish to understand the localization of the state $\psi(t) = \exp(-\frac{it}{\hbar}\hat{H})\eta_\varepsilon$ for relatively long times, of order $|\log\hbar|$. This localization can be measured by taking averages on observables:

$$< A > (\varepsilon, t) :=< \hat{A}\psi(t), \psi(t) > .$$

We shall use the $\hbar$-Weyl quantization defined for $A \in \mathcal{S}(\mathbb{R}^2)$ (the space of Schwartz functions) by the following formula, with $\psi \in \mathcal{S}(\mathbb{R})$,

$$Op_\hbar^w[A]\psi(q) := \hat{A}\psi(q) := \iint_{\mathbb{R}^2} A\left(\frac{q+y}{2}, p\right) \mathrm{e}^{i\frac{\langle x-y,p\rangle}{\hbar}}\psi(y)\frac{dydp}{2\pi\hbar}.$$

Recall that the map $A \mapsto< \hat{A}\psi(t), \psi(t) >$ defines signed measures $\mu_{\hbar,\varepsilon,t}$ on the phase space (Wigner measures) depending on the parameters $\hbar, \varepsilon$ and t. Our goal here is to study the asymptotice behaviour of these measures when

$$\Delta = \max\{\epsilon, \frac{\hbar}{\epsilon}\} \to 0,$$

and for t large and to identify different regimes for their behaviour in the t-$\hbar$ plane.

Let us now describe our results in the particular case where η_ϵ is a coherent state, *i.e.* when $\varepsilon = \sqrt{\hbar}$. If W_ε denotes the Wigner transform of η_ϵ we have

$$< A > (\varepsilon, t) = (2\pi\hbar)^{-1} \int_{\mathbb{R}^2} A(\hbar, t, X) W_\varepsilon(X) dX. \quad (3)$$

Here $A(\hbar, t, X)$ is the Weyl symbol of $\hat{A}(t)$. Using the well known formula [F] $W_\varepsilon(X) = 2\exp(-\frac{|X|^2}{\varepsilon^2})$ this becomes

$$< A > (\varepsilon, t) = \frac{1}{\pi\varepsilon^2} \int_{\mathbb{R}^2} A(\hbar, t, X) \exp(-\frac{|X|^2}{\varepsilon^2}) dX.$$

It is well known from the semi-classical Egorov theorem that

$$A(\hbar, t, X) = A(\Phi_H^t(X)) + R(\hbar, t, X),$$

where $\Phi_H^t(X)$ is the classical Hamiltonian flow defined by the vector field $\left(\frac{\partial H}{\partial p}, -\frac{\partial H}{\partial q}\right)$, and where the remainder term $R(\hbar, t, X)$ is $O_t(\hbar)$ (under suitable assumptions, see for example [R] or [BR]). As a result, one easily sees that for finite times

$$\lim_{\varepsilon \to 0} < A > (\varepsilon, t) = A(\Phi_H^t(X_0)) = A(X_0),$$

since X_0 is a fixed point of the classical dynamics, so that the measures $\mu_{\hbar,\epsilon,t}$ $(\epsilon = \sqrt{\hbar})$ tend to the Dirac measure δ_{X_0}.

Let us now give an idea of what we shall prove in this paper for times t that tend to infinity as $\hbar$ tends to 0, logarithmically in $\hbar^{-1}$. We refer to Theorems 2.1-2.2-2.3 -2.4 for precise statements. Let us assume – to fix ideas – that V is confining and has exactly 3 non-degenerate maxima: $q_- < 0 < q_+$ with $V(0) = V(q_\pm) = 0, V''(0) = -\omega_0^2, V''(q_\pm) = \omega_\pm$ and $V(q) < 0$ for $q \in]q_-, 0[\cup]0, q_+[$ (see Fig. 1). In the following discussion, we suppose for simplicity that $\omega_\pm = \omega_0$. Then there exists a critical time scale $T(\hbar) = \frac{1}{2\omega_0}|\log\hbar|$ such that for $\hbar \to 0$ the following is true:

- If $0 \le t << T(\hbar)$ then $\mu_{\hbar,t} \to \delta_{(0,0)}$;
- If $T(\hbar) << t << \frac{4}{3}T(\hbar)$ then $\mu_{\hbar,t} \to \frac{1}{2}(\delta_{(q_-,0)} + \delta_{(q_+,0)})$;
- If $t \approx T(\hbar)$ then $\mu_{\hbar,t} \to g(X)d\Sigma_0(X)$, where Σ_0 is the 0-energy curve (Fig. 2),

  $$\Sigma_0 = \{X = (q,p), \ \ p^2/2 + V(q) = 0\}$$

  and g is a smooth positive density supported on the unstable part of Σ_0 joining $(q_-, 0)$ to $(q_+, 0)$.

Here and in what follows, $t << T(\hbar)$ means that, for all $\epsilon > 0$, $t \leq (1-\epsilon)T(\hbar)$; the convergence as $\hbar \to 0$ is of course not uniform with respect to ϵ. It is clear that such results can only be obtained by controlling the error term in the Egorov theorem for long enough times. In particular, to observe the transition in the behaviour of $\mu_{\hbar,t}$ at $T(\hbar)$, one needs such control up to times $\beta|\log\hbar|$, for $\beta > \frac{1}{2\omega_0}$. We shall combine techniques developed in [BR] with precise estimates on the flow of H close to the zero-energy curve to control the error for times up to $\frac{2}{3\omega_0}|\log\hbar|$ (Proposition 3.2).

Intuitively, it is not too difficult to convince oneself that a coherent state located initially in $q = 0 = p$ and which therefore has a microlocal support in phase space that is concentrated in a region of size $\sqrt{\hbar}$ around this point, will explore the macroscopic region of phase space that extends up to the nearest neighbours $q_\pm$ at times $t >> \frac{1}{2\omega_0}|\log\hbar|$. This intuition will be further explained below, but it is corroborated by the second statement above. We remark that previous efforts to estimate the evolution of coherent states (in particular Combescure-Robert [CR] and Hagedorn-Joye [HJ]) have concentrated on constructing good semi-classical L^2-approximations of the evolved state. This yields much more detailed information on the state than is needed here since we only study the expectation values of Weyl-quantized classical observables. As a counterpart, the available results on L^2-estimates are valid only up to times $\frac{1}{6\omega_0}|\log\hbar|$, during which the microlocal support of the initial state does not reach a macroscopic size, and they can therefore not be used to obtain the above results. This restriction on the time is related to the observation that, in [CR] [HJ], only the linearized dynamics close to $X_0 = (0,0)$ is used in the analysis. For the longer times we explore here, this is insufficient.

A similar transition in the behaviour of $\mu_{\hbar,\epsilon,t}$ ($\epsilon = \sqrt{\hbar}$) at $T(\hbar)$ was shown in the context of a simple chaotic Hamiltonian system on the two-torus in [BDB1][BDB2]. In that case the $\mu_{\hbar,\epsilon,t}$ converge to the Lebesgue measure for $T(\hbar) << t << 3T(\hbar)$. Roughly speaking, this is due to the fact that in that case, the trajectories starting a distance $\sqrt{\hbar}$ away from the origin explore all of phase space on the time scale considered, due to the exponential mixing of the dynamics. In the present situation, such trajectories converge either to q_+ or to q_-, leading to the second result above.

For coherent states we have $\varepsilon \sim \frac{\hbar}{\varepsilon}$. For a deeper understanding of the phenomena described in this paper it is useful to consider a weaker localization condition on the state η_ε and to work with the two scale paramaters $\hbar, \varepsilon$ independently. By considering initial states in which $\varepsilon << \frac{\hbar}{\varepsilon}$, we will show (Theorem 2.3) that on the same time scale as the one considered above (*i.e.* $t \leq \frac{2}{3\omega_0}|\log\hbar|$), the state explores basically the entire zero-energy surface, as we now explain.

We consider an arbitrary (not necessarily Gaussian) profile φ in the Schwartz space $\mathcal{S}(\mathbb{R})$ such that $\int_{\mathbb{R}} |\varphi(q)|^2 dq = 1$ and define the following normalized state, localized at the origin $(0,0)$ of the phase space,

$$\eta_\varepsilon(q) = \frac{1}{\varepsilon^{1/2}}\varphi\left(\frac{q}{\varepsilon}\right). \tag{4}$$

Hence

$$< \hat{A}(t)\eta_\varepsilon, \eta_\varepsilon >= \int_{\mathbb{R}^2} A(X)d\mu_{\hbar,\varepsilon,t}(X) = \int_{\mathbb{R}^2} A(\hbar,t,X)W_\varphi\left(\frac{q}{\varepsilon}, \frac{\varepsilon}{\hbar}p\right)\frac{dX}{2\pi\hbar},$$

where W_φ is the Wigner function of φ (computed with $\hbar = 1$) and where, by definition, $A(\hbar, t, X)$ is the Weyl-symbol of $\hat{A}(t)$. More generally, we could also consider semi-classical measures $\mu_{\hbar,\varepsilon,t}$ defined by a density matrix $\hat{\rho}_{\hbar,\epsilon}$ with $\rho_{\hbar,\epsilon}(X) = \rho(\frac{q}{\varepsilon}, \frac{\varepsilon}{\hbar}p)$ for some $\rho \in \mathcal{S}(\mathbb{R}^2)$ as follows

$$\int_{\mathbb{R}^2} A(X) d\mu_{\hbar,\varepsilon,t}(X) = \mathrm{Tr}[\hat{A}(t)\hat{\rho}_{\hbar,\varepsilon}] = \int_{\mathbb{R}^2} A(\hbar, t, X)\rho\left(\frac{q}{\varepsilon}, \frac{\varepsilon}{\hbar}p\right)\frac{dX}{2\pi\hbar}.$$

Note that for the states in (4) the Wigner function has a spread Δq in the q-direction given by $\Delta q \sim \varepsilon$, and a spread $\Delta p \sim \frac{\hbar}{\varepsilon}$ in the p-direction. Defining

$$\Delta = \max\{\Delta q, \Delta p\} := \max\{\varepsilon, \frac{\hbar}{\varepsilon}\}, \tag{5}$$

we are interested in the regime where $\Delta \to 0$, so that both ε and $\frac{\hbar}{\varepsilon}$ tend to zero. Clearly

$$\Delta^2 \geq \hbar \tag{6}$$

which is an expression of the Heisenberg Uncertainty Principle. Note that $\Delta \to 0$ implies $\hbar \to 0$. We wish to study $\langle \eta_\varepsilon, \hat{A}(t)\eta_\varepsilon \rangle$ for t as large as possible. For that purpose, we shall start, in Section 3 (Proposition 3.7) by proving that

$$\langle \eta_\varepsilon, \hat{A}(t)\eta_\varepsilon \rangle = \int\int_{\mathbb{R}^2} (A \circ \Phi_H^t)(X)\rho(\frac{q}{\varepsilon}, \frac{\varepsilon}{\hbar}p)\frac{dqdp}{2\pi\hbar} + O(\Delta^s), \tag{7}$$

for some $s > 0$, for all $\Delta \leq \Delta_0$, and, most importantly, for all times t

$$|t| << \frac{2}{3\omega_0}|\log \hbar|. \tag{8}$$

Since it is the goal of semi-classical analysis not only to describe quantum objects in terms of semi-classical ones, but also to extract useful information from the latter, the problem is now reduced to studying the asymptotic behaviour of the first term in the right-hand side of (7). The latter depends on the details of the classical flow for the times in the window (8) and for initial conditions inside a box of size Δ around $(0, 0)$, as $\Delta \to 0$. This study will be done in Section 4.

To understand intuitively what happens, one can assume

$$H(X) = \frac{1}{2}(p^2 - \omega_0^2 q^2)$$

for X in a small neighbourhood of $(0, 0)$. Now, if $|X| \leq \Delta$, then $|\Phi_H^t(X)| \leq e^{\omega_0|t|}\Delta$, so as long as

$$|t| << T_\Delta = \frac{1}{\omega_0}|\log \Delta| \leq \frac{1}{2\omega_0}|\log \hbar|,$$

$|\Phi_H^t(X)| \to 0$ as $\Delta \to 0$, so we expect that

$$\langle \eta_\varepsilon, \hat{A}(t)\eta_\varepsilon \rangle \to A(0, 0),$$

which is indeed correct (Theorem 2.1(i)). To understand what happens for slightly longer times $t = (1+\beta)\frac{|\log\Delta|}{\omega_0}$, one has to remark first that essentially only points X a distance Δ away from 0 contribute effectively to the integral in (7). (This is made precise in Lemma 3.6.) But after a time $\frac{|\log\Delta|}{\omega_0}$ such points have reached a macroscopic distance $e^{\omega_0 t}\Delta \sim 1$ away from the origin, along the unstable manifold, either in the direction of q_-, or of q_+, depending to which sector Ω_i of the plane they belong (see Fig. 2):

- $\Omega_I = \{(q,p),\ H(q,p) < 0,\ q > 0\}, \Omega_{II} = \{(q,p),\ H(q,p) > 0,\ p > 0\}$,
- $\Omega_{III} = \{(q,p),\ H(q,p) < 0,\ q < 0\}, \Omega_{IV} = \{(q,p),\ H(q,p) > 0,\ p < 0\}$.

As long as $\beta \leq 1$, the extra time $\beta\frac{|\log\Delta|}{\omega_0}$ serves those points to reach a distance Δ^β from either q_+ or q_-. For longer times $\beta \geq 1$, they in turn start leaving the neighbourhood of $q_\pm$, reaching a macroscopic distance from those points at a time roughly equal to $3T_\Delta$. This yields for

$$T_\Delta << |t| << 3T_\Delta$$

that

$$\langle \eta_\varepsilon, \hat{A}(t)\eta_\varepsilon\rangle \to (\alpha_I + \alpha_{II})A(q_+) + (\alpha_{III} + \alpha_{IV})A(q_-),$$

where α_i is the fraction of the total mass of the state living in Ω_i:

$$\alpha_i = \lim_{\Delta\to 0} \frac{1}{2\pi\hbar}\iint_{\Omega_i} \rho(\frac{q}{\varepsilon}, \frac{\varepsilon}{\hbar}p)dqdp. \tag{9}$$

Of course, the result holds only for $|t| \leq \frac{2}{3\omega_0}|\log\hbar|$. A precise statement is given in Theorem 2.1 (ii). The mechanism for controlling the first term in the right-hand side of (7) is now clear: for times longer than $3T_\Delta$, the trajectories that started originally at a distance Δ from the origin start escaping to further barrier tops of the potential. The corresponding results on the behaviour of $\langle \eta_\varepsilon, \hat{A}(t)\eta_\varepsilon\rangle$ can be found in Theorem 2.3.

The rest of the paper is organized as follows. In Section 2 we give a detailed statement of our assumptions and results. Section 3 is devoted to the proof of (7), and Section 4 to the control of the classical flow yielding the proofs of the main theorems.

2 Assumptions and Results

We first consider the Hamiltonian $\hat{H} := -\frac{\hbar^2}{2}\frac{d^2}{dq^2} + V$ where V is a triple well potential that satisfies the following assumptions:

(H1) $V \in C^\infty(\mathbb{R})$ and for every $k \in \mathbb{N}$ there exists $C_k > 0$, $M_k \in \mathbb{R}$ such that

$$\left|\frac{d^k V(q)}{dq^k}\right| \leq C_k(1+|q|)^{M_k}$$

(H2) There exist $q_- < 0 < q_+$ such that

(i) $V(0) = V(q_\pm) = 0$, $V(q) < 0$ for every $q \in]q_-, 0[\cup]0, q_+[$.

(ii) $V'(0) = V'(q_\pm) = 0$, $V''(0) = -\omega_0^2$, $V''(q_\pm) = -\omega_\pm^2$, where $\omega_0 > 0$, $\omega_\pm > 0$.

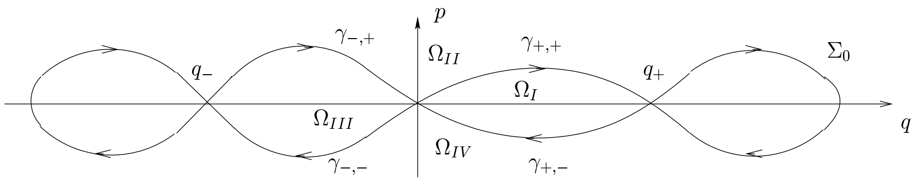

Figure 2: The phase portrait for a quadruple well potential.

Let us denote by $X_j = (q_j, 0)$ the above non-degenerate critical points of H for $j = 0, \pm$. We are interested in a neighborhood in the phase space of the curve

$$\Sigma_0' = \{X = (q, p),\ \ p^2/2 + V(q) = 0,\ q_- \le q \le q_+\}.$$

Obviously (see Fig. 2) $\Sigma_0' \backslash \{X_0, X_-, X_+\}$ is split into 4 branches $\gamma_{+,+}$, $\gamma_{-,-}$, $\gamma_{+,-}$, $\gamma_{-,+}$, where the first index refers to the sign of the q-component and the second index to the sign of the p-component. Moreover $\Sigma_{ust} := \gamma_{+,+} \cup \gamma_{-,-}$ and $\Sigma_{st} := \gamma_{-,+} \cup \gamma_{+,-}$ are respectively the unstable component and the stable component of the energy curve Σ_0'. In particular we have $\lim\limits_{t\to+\infty} \Phi_H^t(X) = X_0$ for $X \in \Sigma_{st}$ and $\lim\limits_{t\to+\infty} \Phi_H^t(X) = X_+$ (respectively X_-) for $X \in \gamma_{+,+}$ (respectively $X \in \gamma_{-,-}$).

Now we can formulate our first main result.

Theorem 2.1 *Let us assume that* (H1) *and* (H2) *hold and let us introduce* $T_\Delta^{(j)} = \frac{|\log\Delta|}{\omega_j}$, $(j = 0\pm)$. *Let* $\omega = \max\{\omega_+, \omega_0, \omega_-\}$. *Let* $A \in \mathcal{S}(\mathbb{R}^2)$, $\epsilon > 0$ *and suppose*

$$|t| \le \frac{2}{3\omega}(1-\epsilon)|\log\hbar|. \tag{10}$$

(i) Let $0 < \delta_1 < 1$ *and suppose in addition to (10) that* $|t| \le (1-\delta_1)T_\Delta^{(0)}$. *Then*

$$\lim_{\Delta\to 0} < \hat{A}(t)\eta_\varepsilon, \eta_\varepsilon >= A(X_0). \tag{11}$$

(ii) Let $0 < \delta_1, \delta_2$ *be small enough and suppose in addition to (10) that*

$$(1+\delta_1)T_\Delta^{(0)} \le t \le T_\Delta^{(0)} + (2-\delta_2)\min\{T_\Delta^{(-)}, T_\Delta^{(+)}\}. \tag{12}$$

Then

$$\lim_{\Delta\to 0} < \hat{A}(t)\eta_\varepsilon, \eta_\varepsilon >= (\alpha_I + \alpha_{II})A(X_+) + (\alpha_{III} + \alpha_{IV})A(X_-). \tag{13}$$

The restriction (10) on the times comes from the control on the error term in the Egorov theorem (Proposition 3.2). The two parts of the theorem correspond to two different regimes in the behaviour of the right-hand side of (7). For part (ii) to be non-trivial, we need of course that

$$\frac{1}{\omega_0}|\log\Delta| < \frac{2}{3\omega}|\log\hbar|, \text{ or } \Delta > \hbar^{\frac{2\omega_0}{3\omega}}.$$

This can be seen as a restriction on Δ, given $\omega_0, \omega_\pm$, or as a restriction on the ω_j, given Δ. For example, for coherent states, where $\Delta = \sqrt{\hbar}$, this yields $4\omega_0 > 3\omega$, which is satisfied in particular when $\omega_\pm = \omega_0$.

As explained in the introduction, these results can be understood by recalling that the initial state lives in a region of phase space of linear size Δ around the origin. This region is stretched to linear size $L_t = \mathrm{e}^{\omega_0 t}\Delta$ in a time t due the instability of the dynamics around $X_0 = 0$. As a result, for times shorter than $\frac{|\log\Delta|}{\omega_0}$, this size tends to 0 as $\Delta \to 0$ and the evolved state therefore still concentrates around X_0. But for the longer times considered in the second part of the Theorem this is no longer correct and the trajectories starting at a distance Δ now reach the neighbouring barrier top $X_\pm$, leading to the second result.

It is also possible to describe in detail what happens on the transition time scale when t is of order $\frac{1}{\omega_0}|\log\Delta|$. As expected, the state then stretches out along the unstable manifold of X_0:

Theorem 2.2 *Let us assume* (H1) *and* (H2). *Suppose that the times t satisfy, in addition to (10),* $\lim_{\Delta\to 0}\Delta\mathrm{e}^{\omega_0 t} = \kappa > 0$ *and that* $\lim_{\varepsilon\to 0}\frac{\hbar}{\varepsilon^\mu} = c$ *for some* $c > 0$ *and some* $\mu \in]1, +\infty[$. *Then there exists a positive smooth density $g_{\kappa,c,\mu}$ on Σ_{ust} such that*

$$\lim_{\Delta\to 0} < \hat{A}(t)\eta_\varepsilon, \eta_\varepsilon >= \int_{\Sigma_{ust}} A(X) g_{\kappa,c,\mu}(X) d\Sigma_0(X),$$

for every observable $A \in C_0^\infty(\mathbb{R}^2)$ such that $supp(A) \subset \{(q,p);\ q_- < q < q_+\}$. Here $d\Sigma_0(X)$ is the flow-invariant Liouville measure on Σ_0. Moreover we can compute $g_{\kappa,c,\mu}$, in position coordinates q, by the following formulae:

$$\begin{aligned} g_{\kappa,c,\mu}(q,p(q)) &= \omega_0 \ell(q) G_{\kappa,c,\mu}(\ell(q)), \quad \text{where} \\ \ell(q) &= \frac{|q|}{\sqrt{2}} \exp\left(\pm \int_0^q \left(\frac{\omega_0}{\sqrt{-2V(u)}} - \frac{1}{u}\right) du\right) \end{aligned}$$

where $\pm$ is $+1$ if $q > 0$ and -1 if $q < 0$. $G_{\kappa,c,\mu}$ is given by the following formulae:

- *First, for the "symmetric" case, where $\mu = 2$ we have*

$$G_{\kappa,c,2}(u) = \frac{1}{2\pi\kappa^2}\int_{\mathbb{R}} \rho\left(\frac{1}{\sqrt{2}\kappa}(u + c\omega_0 v), \frac{1}{\sqrt{2}\kappa}(v - \frac{u}{c\omega_0})\right) dv. \tag{14}$$

- *For $2 < \mu < +\infty$ we have*

$$G_{\kappa,c,\mu}(u) = \frac{\sqrt{2}}{\kappa\pi}\int_{\mathbb{R}} \rho\left(\frac{\sqrt{2}}{\kappa}u, v\right) dv.$$

- *For* $0 < \mu < 2$ *we have*

$$G_{\kappa,c,\mu}(u) = \frac{\sqrt{2}}{\kappa\pi\omega}\int_{\mathbb{R}} \rho\left(v, -\frac{\sqrt{2}}{\kappa}u\right) dv.$$

Let us remark that the density above is defined for $q_- < q < q_+$ and is positive except at 0 where it vanishes so that it is integrable for the Liouville measure on Σ_{ust}, $d\Sigma(q, p(q)) = \frac{dq}{\sqrt{p(q)}}$ where $p(q) = \pm\sqrt{-2V(q)}$ describes the unstable part of the 0-energy curve. Moreover let us remark that for $\rho = W_\varphi$, G is given more explicitly in term of φ or its Fourier transform $\tilde{\varphi}$ using the well known formulae

$$\int_{\mathbb{R}} W_\varphi(u,v)dv = 2\pi|\varphi(u)|^2, \ \int_{\mathbb{R}} W_\varphi(u,v)du = |\tilde{\varphi}(u)|^2.$$

We now turn to what happens for times longer than $3T_\Delta$. For that purpose, it is of interest to consider also the case when there are more barrier tops. We will consider three types of potentials.

First, we consider confining multiple well potentials with $N_- + N_+ + 1$ barrier tops ($N_\pm \in \mathbb{N}$). The case of a confining potential with a total of 4 barrier tops is drawn in Fig. 3. The precise assumptions on V are in this case:

(H3) There exist $-\infty < q_{-N_- -1} < q_{-N_-} < \cdots < q_0 = 0 < \cdots < q_{N_+} < q_{N_+ +1}$ ($N_\pm \in \mathbb{N}$) such that:

(i) $V(q_j) = 0$ for all $-N_- \leq j \leq N_+$ and $V(q) < 0$ for all $q \in]q_{-N_- -1}, q_{N_+ +1}[$, $q \neq q_j$;

(ii) $V'(q_j) = 0$ for all $-N_- \leq j \leq N_+$;

(iii) $V''(q_j) = -\omega_j^2 < 0$ for all $-N_- \leq j \leq N_+$.

(iv) $V(q_{-N_- -1}) = 0 = V(q_{N_+ +1})$, $V'(q_{-N_- -1}) < 0$, $V'(q_{N_+ +1}) > 0$ and $V(q) > 0$ for all $q > q_{N_+ +1}, q \leq q_{-N_- -1}$.

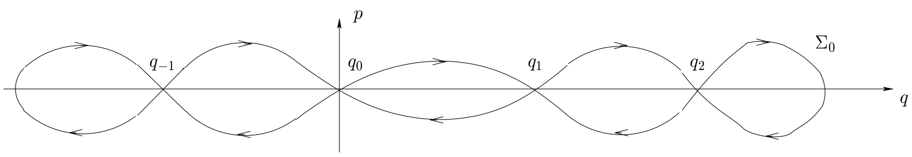

Figure 3: Phase portrait of a confining 5-well potential with $N_+ = 2, N_- = 1$.

Our results also hold for potentials with an infinite number of wells, such as periodic potentials. In that case, the precise conditions on V are:

(H4) There exists $\delta > 0$ and a sequence $q_j, j \in \mathbb{Z}$, $q_{j+1} - q_j > \delta$, $q_0 = 0$ such that $V(q_j) = 0 = V'(q_j)$, and $V''(q_j) = -\omega_j^2 < 0$. Moreover, $V(q) < 0$ if $q \neq q_j$ and

$$0 < \inf \omega_j \leq \sup \omega_j < +\infty.$$

Finally, we can also deal with non-confining multiple well potentials (Figure 4):

(H5) There exist $-\infty < q_{-N_--1} < q_{-N_-} < \cdots < q_0 = 0 < \cdots < q_{N_+} < q_{N_++1}$ ($N_\pm \in \mathbb{N}$) such that (H3)(i)-(ii)-(iii) hold and furthermore: there exists $v > 0$ so that, for all $q \geq q_{N_++1}$ and for all $q \leq q_{-N_--1}$, $V(q) \leq -v$.

We can of course also deal with potentials that are confining on one side, and not on the other, and other similar cases. We define

$$\omega = \sup\{\omega_j\} < +\infty. \tag{15}$$

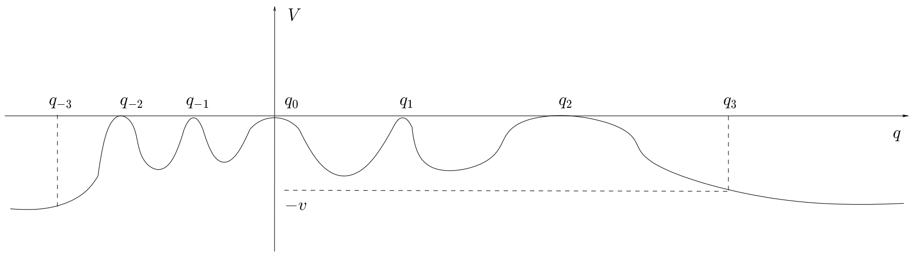

Figure 4: A non-confining 4-well potential with $N_+ = 2 = N_-$.

Theorem 2.3 *Let us assume* **(H1)** *and either* **(H3)**, **(H4)** *or* **(H5)** *hold, with $\omega_j = \omega_0$ for all j. Suppose furthermore that for some $m \geq 1$, we have $0 < \hbar \leq \Delta^{2m}$. Let $k \in \mathbb{N}$ and let $\delta_1, \delta_2 > 0$ be such that $\delta_1 < 2 - \delta_2$ and $2k + 1 - \delta_2 < \frac{4m}{3}$. Let $A \in \mathcal{S}(\mathbb{R}^2)$.*

In case (H5) holds, assume moreover $k \leq N_-, N_+$ and $A \in C_0^\infty(\mathbb{R}^2)$.

Then, as long as t stays in the interval $[(2\ell - 1 + \delta_1)T_\Delta^{(0)}, (2\ell + 1 - \delta_2)T_\Delta^{(0)}]$ for some $0 \leq \ell \leq k$, there exist four critical points $X_{j(\ell,i)}$ such that for all $A \in C_0^\infty(\mathbb{R}^2)$

$$\lim_{\varepsilon \to 0} < \hat{A}(t)\eta_\varepsilon, \eta_\varepsilon >= \sum_{i=I}^{IV} \alpha_i A(X_{j(\ell,i)}),$$

where the α_i are defined in (9).

It is actually not difficult to identify the indices $j(\ell, i)$ for small enough ℓ. If (H3) or (H5) hold and if $\ell \leq N_-, N_+$, or if (H4) holds and if $\ell \in \mathbb{N}$, we have:

- If ℓ is even,

$$\lim_{\varepsilon \to 0} < \hat{A}(t)\eta_\varepsilon, \eta_\varepsilon >= (\alpha_I + \alpha_{III})A(X_0) + \alpha_{II}A(X_\ell) + \alpha_{IV}A(X_{-\ell}); \tag{16}$$

- If ℓ is odd,

$$\lim_{\varepsilon\to 0} < \hat{A}(t)\eta_\varepsilon, \eta_\varepsilon >= \alpha_I A(X_1) + \alpha_{III} A(X_{-1}) + \alpha_{II} A(X_\ell) + \alpha_{IV} A(X_{-\ell}). \tag{17}$$

Similar statements can be made when the ω_j are distinct, but they are considerably messier because the time scales are more complicated to describe. A less precise statement that is easily formulated is the following.

Theorem 2.4 *Let us assume that* **(H1)** *and either* **(H3)** *or* **(H4)** *hold. Let $\tau_* = \frac{2}{3\omega}$. Then, there exists, for all $\delta > 0$, a subset $I \subset [-\tau_*, \tau_*]$ such that*

(i) $|I| = (2\tau_* - \delta)$.

(ii) For all $\tau \in I$, there exist four critical points $X_{j(\tau,i)}$ such that for all $A \in \mathcal{S}(\mathbb{R}^2)$,

$$\lim_{\varepsilon\to 0} < \hat{A}(\tau|\log\hbar|)\eta_\varepsilon, \eta_\varepsilon >= \sum_{i=I}^{IV} \alpha_i A(X_{j(\tau,i)}),$$

where the α_i are defined in (9).

Theorem 2.4 can be paraphrased by saying that "most of the time" the semi-classical measures $\mu_{\hbar,\epsilon,t}$ converge to a sum of at most four Dirac delta-measures on the critical points X_j. The set I is in fact a finite union of intervals.

Theorem 2.3 shows the occurrence of intervals of time of length $2T_\Delta^{(0)}$ centered at even multiples of $T_\Delta^{(0)}$. First, as in part (i) of Theorem 2.1 one sees that for times t between $-T_\Delta^{(0)}$ and $T_\Delta^{(0)}$ (*i.e.* $\ell = 0$) the particle stays close to 0. Next, as will be seen in Section 4 (see also the informal discussion in the introduction), the time needed to go with the classical dynamics along the energy curve $\Sigma_{\Delta^2} := \{|H(q,p)| = \Delta^2\}$ from some neighborhood of X_0 to a neighborhood of X_1 or X_{-1} is slightly longer than $T_\Delta^{(0)}$. Once the particle has come close to one of these two points, it stays again a period $2T_\Delta^{(0)}$ close to them, before exploring further barrier tops ($\ell > 1$) starting at $t = 3T_\Delta^{(0)}$. In general, it will therefore approach the ℓ-th top away from 0 at times slightly longer than $(2\ell+1)T_\Delta^{(0)}$. This helps to explain the formulas (16)-(17).

Now, as pointed out in the introduction, under the hypotheses of Theorem 2.3, we can control the quantum dynamics only up to times $\frac{2}{3\omega_0}|\log\hbar|$. So, for the particle to reach the ℓ-th top in this time, one needs

$$\Delta^{\frac{3(2\ell+1)}{2}} \geq \hbar,$$

which explains the origin of the condition on k and m in the hypotheses of Theorem 2.3. In particular, if we choose $\Delta = \varepsilon = \sqrt{\hbar}$ (*i.e.* $m = 1$), as for coherent states, then the wavefunction only visits the sites $X_\pm$ in the allowed time scale and Theorem 2.3 reduces to Theorem 2.1. Only if $m > 1$ do we obtain new results.

Let us finally remark that, when $m > 1$, we have two regimes : either $\Delta = \frac{\hbar}{\epsilon} << \epsilon$, where the spread of the Wigner function is larger in the q-direction than in the p-direction or $\Delta = \frac{\hbar}{\epsilon} >> \epsilon$, where the spread of the Wigner function is larger in the

p-direction than in the q-direction. As is easily checked, in the first regime only $\alpha_{I,III}$ are different from zero so that the quantum particle never actually visits the sites X_ℓ and $X_{-\ell}$ ($\ell > 1$) on the time scale considered. The most interesting case is therefore the second regime.

In conclusion, our result in Theorem 2.3 shows that the initial state, essentially supported in four small neighborhoods C_i near X_0 located inside Ω_i, for $i = I, II, III, IV$, is carried by the time evolution into 4 different small neighbourhoods of one of the critical points X_j. The components C_I and C_{III} are oscillating between X_0 and $X_\pm$, whereas C_{II} and C_{IV} are moving in the clockwise direction along the 0 energy curve. A new macroscopic distribution of the total mass of the initial state occurs at each approximate period of time $(2\ell+1)T_\Delta$ (transition times). Actually, if the potential is confining, as in Fig. 3, for example, we can easily follow the evolution of $\mu_{\hbar,\varepsilon,t}$ when the state makes loops around Σ_0.

As in Theorem 2.2, we could also describe what happens at the transition times $(2\ell+1)T_\Delta^{(0)}$ in terms of absolutely continuous measures on unstable curves, assuming the condition $\lim\limits_{\Delta\to 0} \Delta^{2\ell+1} \mathrm{e}^{\omega_0 t} = \kappa > 0$.

3 Reduction to a classical estimate

Our goal in this section is to prove (7), or, more precisely, Proposition 3.7. Let us assume that (H1) and either (H3), (H4) or (H5) are satisfied, together with (15). Let χ be a smooth function with compact support such that $\chi(u) = 1$ for $|u| \le 2$. In order to localize close to the energy 0, let us introduce the observable

$$\widehat{B_E} := \chi\left(\frac{\hat{H}}{E}\right)\hat{A}\chi\left(\frac{\hat{H}}{E}\right).$$

¿From now on it is understood that $A \in \mathcal{S}(\mathbb{R}^2)$, unless we work under hypothesis (H5), in which case $A \in C_0^\infty(\mathbb{R}^2)$. Then we have first of all:

Proposition 3.1 *For every $a > 0$, every $N > 0$, there exist $C_1 > 0$, $C_2 > 0$, such that for all $t \in \mathbb{R}$*

$$\left| < \hat{A}(t)\eta_\varepsilon, \eta_\varepsilon > - < \widehat{B_E}(t)\eta_\varepsilon, \eta_\varepsilon > \right| \le C_1 \frac{\hbar}{E} + C_2 \left(\frac{\Delta}{\sqrt{E}}\right)^N \tag{18}$$

for every $E \le a$, $\Delta \le a\sqrt{E}$.

The following result then shows that the main contribution to $< \hat{A}(t)\eta_\varepsilon, \eta_\varepsilon >$ comes from the evolution of the principal (classical) term defined by

$$B_{E,0}(X) := \chi^2\left(\frac{H(X)}{E}\right)A(X), \quad B_{E,0}(t) = B_{E,0} \circ \Phi_H^t.$$

Proposition 3.2 *For every $\delta > 0$ and every $a > 0$ there exist $C_1 > 0$, $C_2 > 0$, $s > 0$ such that*

$$\left| < (\widehat{B_E}(t) - Op_\hbar^w B_{E,0}(t))\eta_\varepsilon, \eta_\varepsilon > \right| \le C_1 \hbar^s + C_2 \frac{\hbar^2}{E^3} \tag{19}$$

for every $|t| \leq \frac{2-3\delta}{3\omega}|\log(\hbar)|$, $\hbar \leq a$, $\hbar^2 \leq aE^3$.

It is not difficult to see that Proposition 3.1 results directly from the following lemma.

Lemma 3.3 *For every* $N > 0$*, every* $a > 0$ *there exist* $C_1 > 0$*,* $C_2 > 0$ *such that*

$$\left\| \chi\left(\frac{\hat{H}}{E}\right)\eta_\varepsilon - \eta_\varepsilon \right\| \leq C_1\frac{\hbar}{E} + C_2\left(\frac{\Delta}{\sqrt{E}}\right)^N \tag{20}$$

for every $\Delta \leq a\sqrt{E}$*,* $E \leq a$.

Proof of Lemma 3.3: Using the functional calculus for pseudodifferential operators depending on parameters (see for example [DR]), we have

$$\left(I - \chi\left(\frac{\hat{H}}{E}\right)\right)^2 = Op_\hbar^w\left(1 - \chi\left(\frac{H}{E}\right)\right)^2 + O(\frac{\hbar}{E}).$$

But, using the Wigner function of η_ε we have

$$< Op_\hbar^w\left(1-\chi\left(\frac{H}{\varepsilon}\right)\right)^2\eta_\varepsilon, \eta_\varepsilon >= \int_{\mathbb{R}^2}\left(1-\chi\left(\frac{H(q,p)}{E}\right)\right)^2\rho\left(\frac{q}{\varepsilon}, p\frac{\varepsilon}{\hbar}\right)\frac{dqdp}{2\pi\hbar},$$

so that we have to estimate

$$F(E,\hbar) := \int_{[|H(q,p)|\geq E]}\left|\rho\left(\frac{q}{\varepsilon}, p\frac{\varepsilon}{\hbar}\right)\right| dqdp.$$

Because ρ is fast decreasing at ∞ we have for every $\theta \in]0,1[$,

$$\int\int_{[|q|+|p|\geq\Delta^\theta]}\left|\rho\left(\frac{q}{\varepsilon}, p\frac{\varepsilon}{\hbar}\right)\right| dqdp = O(\Delta^{+\infty}).$$

But close to 0 we can use the Taylor formula:

$$H(q,p) = \frac{1}{2}\left(p^2 - \omega_0^2 q^2\right) + O(|q|^3 + |p|^3)$$

and we have for $\Delta^{3\theta} \leq cE$ with $c > 0$ small enough,

$$F(E,\hbar) \leq (2\pi\hbar)^{-1}\int\int_{\left[\begin{array}{c}|p^2-\omega^2q^2|\geq E\\ |q|+|p|\leq\Delta^\theta\end{array}\right]}\left|\rho\left(\frac{q}{\varepsilon}, p\frac{\varepsilon}{\hbar}\right)\right| dqdp + O(\Delta^{+\infty}).$$

The conclusion of the lemma will therefore be a consequence of the following estimate: for every ρ in the Schwartz space $\mathcal{S}(\mathbb{R}^2)$ and every $N \geq 1$ we have

$$(2\pi\hbar)^{-1}\int\int_{[|p^2-\omega_0^2q^2|\geq E]}\left|\rho\left(\frac{q}{\varepsilon}, p\frac{\varepsilon}{\hbar}\right)\right| dqdp = O\left(\left(\frac{\Delta}{\sqrt{E}}\right)^N\right) \tag{21}$$

To prove this, we start by the change of variables $q = \varepsilon u$, $p = \frac{\hbar}{\varepsilon}v$ and we introduce $\tilde{E} := \frac{E}{\Delta^2}$. Assuming $\Delta = \epsilon$ (the case where $\Delta = \hbar/\epsilon$ is treated similarly), it is not difficult to see that we have to estimate for $\tilde{E} \to +\infty$, the following integrals depending on the parameter $c \in]0, c_0[$, $c_0 > 0$.

$$I(\tilde{E}, c) = \int_{|c^2p^2 - q^2| \geq \tilde{E}} |\rho(q,p)| dq dp.$$

Considering the two different cases $q^2 \geq \frac{\tilde{E}^2}{4}$ and $q^2 \leq \frac{\tilde{E}^2}{4}$ we get easily, for every $N \geq 1$,

$$I(\tilde{E}, c) = O(\tilde{E}^{-N})$$

uniformly in $c \in]0, c_0[$. This implies (21), and ends the proof of the Lemma, which in turn implies Proposition 3.1. ∎

The proof of Proposition 3.2 will be obtained by adapting the methods of [BR] to Hamiltonions depending on the extra parameter ε. The application of the constructions of [BR] is relatively straightforward because all the terms occurring in that paper are controlled using the size of the derivatives of the (evolved) classical observables. The extra and essential ingredient for the proof of Proposition 3.2 is the following estimate on the classical flow, which will be proved later in this section.

Lemma 3.4 *Let us assume* **(H1)** *and either* **(H3)**, **(H4)** *or* **(H5)**. *Then there exists $E_1 > 0$ such that, for every $\tau > 0, R > 0$, every $\gamma \in \mathbb{N}^2$ there exists $C_{\gamma,\tau,R}$ with the following properties. For every E, $0 < E \leq E_1$, there exists δ_E satisfying $\lim_{E \to 0} \delta_E = 0$ and such that for every X, $|H(X)| \leq E$, we have*

$$\left|\partial_X^\gamma \Phi_H^t(X)\right| \leq C_{\gamma,\tau,R} \exp[(\omega + \delta_E)|\gamma||t|] \tag{22}$$

for all $|t| \leq \tau |\log E|$ and, if (H5) holds, provided $|\Phi_H^{t'}(X)| < R, 0 \leq t' \leq t$.

Proof of Proposition 3.2: Using Lemma 3.4 and working as in [BR] we shall obtain Proposition 3.2. For that purpose we first easily prove the following estimates, using Lemma 3.4,

$$|\partial_X^\gamma B_{E,0}(\Phi_H^t(X))| \leq C_{0,\gamma} \left(E^{|\gamma|} + \exp[(\omega + \delta_E)|\gamma||t|)]\right)$$

where $0 \leq \delta_E$ tends to 0 as E tends to 0. According to [BR], we know that

$$\widehat{B_E}(t) \approx \sum_{\substack{j \geq 0, \\ j \text{ even}}} \hbar^j Op_\hbar^w[B_{E,j}(t)].$$

Using the Leibniz rule and revisiting the proofs of [BR] (in particular Lemma 2.5), one obtains through an induction on j (even) that

$$|\partial_X^\gamma B_{E,j}(t, X)| \leq C_{j,\gamma} \left(E^{-(|\gamma| + 3j/2)} + \exp[(\omega + \delta_E)|t|(|\gamma| + 3j/2)]\right),$$

uniformly in $X, t, E, \hbar$. Now using the accurate remainder estimate for products of observables (see [BR], Appendix and Lemma 3.6) and the Calderon-Vaillancourt theorem we have, for every $N \geq 1$,

$$\|\widehat{B_E(t)} - \sum_{\substack{N \geq j \geq 0, \\ j \text{ even}}} \hbar^j Op_\hbar^w[B_{E,j}(t)]\| \leq$$

$$C_N \hbar^{(N+1)}(1+|t|)^{N+d_1} \left(E^{-(3N/2+d_1)} + \exp[(3N/2+d_1)(\omega+\delta_E)|t|] \right)$$

where $d_1 \leq 8$. Using this estimate, it is now easy to conclude the proof. Indeed, choosing N large enough and E small enough and writing the terms $< Op_\hbar^w[B_{E,j}(t)]\eta_\varepsilon, \eta_\varepsilon >$ for $1 \leq j \leq N$ directly in terms of the Wigner function of η_ϵ, one readily finds (19).
■

Now it remains to prove Lemma 3.4. Under hypothesis (H3), for example, the problem is the following: for non-zero energy E the motion is periodical so the X derivatives of the flow are uniformly bounded in time. But these bounds blow up in time when E goes to zero because the particle goes slower and slower close to the critical points X_j. In the lemma, we prove a bound that is uniform in energy, for times of order $|\log E|$.

A nice way to control what happens in a neighborhood of the critical points is to use suitable normal forms. Let $X_j = (q_j, 0)$ be one of the critical points appearing in the hypotheses. Then we have the following reduction to a normal form for the Hamiltonian H (see [CV, HS] for a proof).

Proposition 3.5 *There exists $\rho > 0$, a smooth symplectic diffeomorphism F_j from $D_{\rho,j} =]q_j - \rho, q_j + \rho[\times] - \rho, \rho[$ into a neighborhood $\tilde{D}_j$ of the origin (0, 0) in $\mathbb{R}^2$ and a smooth function $f_j : H(D_{j,\rho}) \mapsto \mathbb{R}$ with the following properties:*

- $F_j(X_j) = 0$;
- $\forall X \in D_{j,\rho}$ *we have* $(K \circ F_j)(X) = f_j(H(X))$ *where* $K(\tilde{q}, \tilde{p}) = \tilde{q}\tilde{p}$;
- $f_j'(0) = \omega_j^{-1}$, $f_j(0) = 0$;
- $F'(X_j) = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -\omega_j \\ \omega_j^{-1} & 1 \end{pmatrix}$.

In particular we have the following relationship between the flows

$$\Phi^s_{f(H)}(X) = F_j^{-1} \circ \Phi^s_K \circ F_j(X), \tag{23}$$

for all $X \in D_{j,\rho}$ and $s \geq 0$ so that $\Phi^{s'}_{f(H)}(X) \in D_{j,\rho}$ for all $0 \leq s' \leq s$.
Moreover we also have:

- $\Phi^s_{f(H))}(X) = \Phi^t_H(X)$ *with* $t = f'(H(X))s$.

Note that the dynamics of K is explicitly given by $\Phi_K^s(\tilde{q},\tilde{p}) = (e^s\tilde{q}, e^{-s}\tilde{p})$.

Proof of Lemma 3.4: Let us begin with a preliminary remark. If the lemma is proved for some $\tau = \tau_0 > 0$ then we can get the result for every $\tau > 0$. Indeed, using the group property of the flow ($\Phi_H^{t_1+t_2} = \Phi_H^{t_1} \circ \Phi_H^{t_2}$) and an induction on the integer m gives the conclusion of the lemma for $m\tau_0$, for every m.

We shall therefore prove the lemma for $\tau_0 = \frac{1}{\omega}$; the reason is that $\frac{1}{\omega}|\log(E)|$ is less than the time needed to travel accross any one box $D_{\rho/2,j}$ on a path of energy $\pm E$, for E small enough (since $\omega \geq \omega_j$). We first give the proof under conditions (H3) or (H4). Let $\rho > 0$ be fixed and small enough so that the boxes $\{D_{\rho,j},\ -N_- \leq j \leq N_+\}$ do not intersect. In what follows we always assume $t \geq 0$, so t will be increasing, and $E > 0$. (The other cases are similar and will not be given in detail.) As a result, the classical paths are oriented by the time and the notion of consecutive boxes is relative to this ordering. Since $E > 0$, the classical path moves from (the neighbourhood of) one critical point X_j to the next. For confining potentials (condition (H3)), after visiting (a neighbourhood of) X_{N_+}, the path is reflected by the turning point q_{N_++1}, turns to the left to visit X_{N_+} again and then continues on towards X_{N_+-1}, and so on; the same for X_{-N_-1} where, arriving from the left, the particle goes after reflection to the right. Under condition (H4), the particle just keeps going in one direction.

First of all, it is clear that there exists a time T_1 such that, for every $0 \leq E \leq E_1$, the time $t_{1,j}(E)$ it takes to travel along $|H(X)| = E$ between (the edges of) any two consecutive boxes $D_{\rho/2,j}$ and $D_{\rho/2,j+1}$ satisfies $|t_{1,j}(E)| \leq T_1$, and is therefore uniformly bounded for $0 \leq E \leq E_1$. It is clearly sufficient to prove the result for all $t \geq T_1$. We shall consider the following two cases.

1. $X \notin \cup_j \overline{D_{\rho/2,j}}$. In other words, the initial condition is situated somewhere between two consecutive boxes $D_{\rho/2,j_0}$ and $D_{\rho/2,j_0+1}$. Then there exists $t_2(E) \leq t_1(E) \leq T_1$ (we drop the index j_0) such that $\Phi_H^{t_2(E)}(X)$ belongs to the edge of $D_{\rho/2,j_0+1}$. In other words, it takes a finite time less than T_1 for the particle to reach the next box. Let us furthermore remark that the particle is entering the small box $D_{\rho/2,j_0+1}$ at X_{j_0+1} after a time $t_2(E) \leq T_1$ and that it will then stay there for an amount of time of order $\omega_{j_0}^{-1}|\log E| \geq \tau_0|\log E|$. Writing $\Phi_H^t(X) = \Phi_H^{t-t_2(E)}(\Phi_H^{t_2(E)}(X))$, and remarking that $t - t_2(E) \leq \tau_0|\log E|$, we can therefore estimate $\Phi_H^{t-t_2(E)}(Y)$ with $Y = \Phi_H^{t_2}(X)$ which is in $D_{\rho/2,j_0+1}$ using the normal form:

$$\Phi_H^u(Y) = F_{j_0}^{-1} \circ \Phi_K^{u/f'(H(X))}(F_{j_0}(Y)).$$

Hence noticing that $\lim_{E\to 0} f'_{j_0}(E) = \omega_{j_0}^{-1} \geq \omega^{-1}$, we find after some computations

$$\left|\partial_X^\gamma \Phi_H^t(X)\right| \leq C_{\gamma,E_1} \exp[(\omega + \delta_E)|\gamma||t|], \tag{24}$$

for all $|t| \leq \tau_0|\log(E)|$ where $E := |H(X)| \leq E_1$ and $\lim\limits_{E\to 0} \delta_E = 0$.

2. Assume now that $X \in \overline{D_{\rho/2,j_0}}$ for some j_0; in other words, the initial condition is in a small neighbourhood of one of the critical points. There are now two possibilities. Either $\Phi_H^t(X) \in D_{\rho,j_0}$, for all $0 \leq t \leq \tau_0|\log E|$. This means that at the initial value X the trajectory is just "entering" the box $D_{\rho/2,j_0}$ and therefore spends at least a time $\tau_0|\log E|$ before leaving again. In that case one can apply the normal form directly during the entire time span and obtain the result as above. If, on the other hand, there exists $0 < t' < \tau_0|\log E|$ so that $\Phi_H^{t'}(X) \in \partial D_{\rho,j_0}$, so that the trajectory leaves the box D_{ρ,j_0} at a time t' shorter than $\tau_0|\log E|$, then we write $\Phi_H^t(X) = \Phi_H^{t-t'}(\Phi_H^{t'}(X))$. Applying the normal form to $\Phi_H^{t'}(X)$ and part **1.** to control $\Phi_H^{t-t'}(Y)$ with $Y = \Phi_H^{t'}(X)$, the result follows again.

It is not difficult to adapt the above proof to condition (H5). This is where the condition involving R comes into play. Note that the proof goes through unaltered for points X that, in the future, come close to one of the critical points, *i.e.*, such that there exists $t' > 0$ for which $\Phi_H^{t'}(X)$ enters a box $D_{\rho/2,j_0}$, for some j_0. Under conditions (H3) or (H4), this is true for all X with $|H(X)| \leq E_1$. In the case of condition (H5), this is still true for all $X = (q,p)$ with $q_{N_- -1}+\rho < q < q_{N_+ +1}-\rho$, but not necessarily otherwise, since some trajectories escape to infinity. Let us therefore consider the case where $q_{N_+ +1} < q < R$ and call the point X "outgoing" if the trajectory starting at X does not meet the box $D_{\rho/2,N_+}$ in the future or leaves it before $\tau_0|\log E|$. The crucial observation is now that, in that case, it takes at most a finite time T_R to reach $q = R$, uniformly in E; for such initial conditions the estimate is trivial. The same reasoning works for outgoing initial conditions with $q < q_{N_- -1} - \rho$. ■

Until now we have proved that for some $s > 0$, for every $N \geq 1$ we have

$$< \hat{A}(t)\eta_\varepsilon, \eta_\varepsilon > = < Op_\hbar^w[B_{E,0}(t)]\eta_\varepsilon, \eta_\varepsilon > + O\left(\hbar^s + \frac{\hbar^2}{E^3} + \frac{\hbar}{E} + \left(\frac{\Delta}{\sqrt{E}}\right)^N\right),$$

where

$$< Op_\hbar^w[B_{E,0}(t)]\eta_\varepsilon, \eta_\varepsilon > = \iint_{\mathbb{R}^2} \chi^2\left(\frac{H(q,p)}{E}\right) A(\Phi_H^t(q,p))\rho\left(\frac{q}{\varepsilon}, p\frac{\varepsilon}{\hbar}\right)\frac{dqdp}{2\pi\hbar}. \tag{25}$$

The final step is to prove that only energies E between $\Delta^{2+\sigma_1}$ and $\Delta^{2-\sigma_2}$ ($\sigma_j > 0,\ j = 1,\ 2$, arbitrary small) contribute in (25).

Lemma 3.6 *For every $\sigma_1 > 0$, $\sigma_2 > 0$:*

$$\hbar^{-1}\iint_{[|H(q,p)|\leq\Delta^{2+\sigma_1}]}\left|\rho\left(\frac{q}{\varepsilon}, p\frac{\varepsilon}{\hbar}\right)\right| dqdp = O(\Delta^{\sigma_1/2})$$
$$\hbar^{-1}\iint_{[|H(q,p)|\geq\Delta^{2-\sigma_2}]}\left|\rho\left(\frac{q}{\varepsilon}, p\frac{\varepsilon}{\hbar}\right)\right| dqdp = O(\Delta^{+\infty})$$

Proof: The second estimate was already proved in (21). Let us estimate here the integral

$$I(E,\hbar) = \iint_{[|H(q,p)|\leq E]}\left|\rho\left(\frac{q}{\varepsilon}, p\frac{\varepsilon}{\hbar}\right)\right|\frac{dqdp}{\hbar}.$$

Because ρ is fast decreasing it is sufficient to integrate in $|q| \leq \Delta^\theta$ for some $2/3 < \theta < 1$. But in a domain where q is small, we can use the Taylor formula to obtain

$$H(q,p) = \frac{1}{2}(p^2 - \omega_0^2 q^2) + O(q^3),$$

so that it is enough to estimate

$$I_0(E,\hbar) = \iint_{\left[|p^2-\omega_0^2 q^2|\leq 2(E+\Delta^{3\theta})\right]} \left|\rho\left(\frac{q}{\varepsilon}, p\frac{\varepsilon}{\hbar}\right)\right| \frac{dqdp}{\hbar}. \tag{26}$$

Assume now $\Delta = \epsilon$. The other case is treated similarly. We change variables by putting $q = \varepsilon u, p = \frac{\hbar}{\varepsilon} v$ and we introduce $\tilde{E} = \frac{E}{\Delta^2}$, $c = \frac{\hbar}{\Delta^2}$, so that

$$I_0(E,\hbar) \leq \iint_{\left[|c^2v^2-\omega_0^2u^2|\leq 3\tilde{E}\right]} |\rho(u,v)|\, dudv.$$

Splitting the domain of the integral $I_0(E,\hbar)$ into $\{u^2 \leq 4\tilde{E}\}$ and $\{u^2 > 4\tilde{E}\}$ and using $0 < c \leq 1$ (Uncertainty Principle!) we get

$$I_0(E,\hbar) = O(\sqrt{\tilde{E}}), \tag{27}$$

which concludes the proof of Lemma 3.6. ∎

The conclusion of the work done so far can be formulated in the following proposition, which shows that the study of the long-time quantum averages considered in this paper can be reduced to a purely classical long-time analysis.

Proposition 3.7 *For every* $0 < \sigma_1, \sigma_2, \sigma_3 < 1$, $\delta > 0$, $\Delta_0 > 0$ *there exists* $s > 0$ *such that*

$$< \hat{A}(t)\eta_\varepsilon, \eta_\varepsilon >= \iint_{\Omega_\sigma(\Delta)} A(\Phi_H^t(q,p))\rho\left(\frac{q}{\varepsilon}, p\frac{\varepsilon}{\hbar}\right)\frac{dqdp}{2\pi\hbar} + O(\Delta^s)$$

uniformly for $|t| \leq \frac{2-3\delta}{3\omega}|\log(\hbar)|$, $\Delta \leq \Delta_0$. *Here*

$$\Omega_\sigma(\Delta) = \left\{(q,p) \in \mathbb{R}^2, \Delta^{2+\sigma_1} \leq |H(q,p)| \leq \Delta^{2-\sigma_2},\ |q| + |p| \leq \Delta^{1-\sigma_3}\right\}$$

and $\omega = \max\{\omega_j\}$.

4 Controlling the classical flow

Now we can proceed to the proof of Theorems 2.1-2.2-2.3-2.4. In view of the results of the previous section (Proposition 3.7) it remains to study carefully the long time behaviour of the classical trajectories for initial conditions near the critical point X_0.
Proof of Theorem 2.1 (i): Let us recall that $X_0 = (0,0)$. Using the Taylor formula we have, for every $X \in \Omega_\sigma(\Delta)$

$$|A(\Phi_H^t(X)) - A(\Phi_H^t(X_0))| \leq C\Delta^{1-\sigma_3} \sup_{Y\in\Omega_\sigma(\Delta)} |\partial_Y \Phi_H^t(Y)|,$$

where C is independent of t or Δ. For $|t| \leq (1-\delta_1)T_\Delta^{(0)}$ one can use, as in the proof of Lemma 3.4, the normal form close to X_0 to obtain

$$|A(\Phi_H^t(X)) - A(\Phi_H^t(X_0))| \leq C\Delta^{1-\sigma_3}\exp[(\omega_0 + \eta_\Delta)|t|]. \tag{28}$$

where $\eta_\Delta \to 0$ as $\Delta \to 0$. Since σ_3 can be chosen as small as desired the result (i) follows easily from Proposition 3.7. ∎

Proof of Theorem 2.1 (ii): We define $\Omega_\sigma^i(\Delta) = \Omega_i \cap \Omega_\sigma(\Delta)$ where $i = I, II, III, IV$ (Fig. 2). In view of Proposition 3.7, it is clearly enough to show that there exist $0 < \sigma_1, \sigma_2, \sigma_3 < 1$ so that

$$J_\Delta^i(t,\hbar) = (2\pi\hbar)^{-1} \iint_{\Omega_\sigma^i(\Delta)} A(\Phi_H^t(q,p))\rho\left(\frac{q}{\varepsilon}, p\frac{\varepsilon}{\hbar}\right) dqdp,$$

satisfies

$$\lim_{\Delta\to 0} J_\Delta^i(t,\hbar) = \alpha_i A(X_+), i = I, II; \qquad \lim_{\Delta\to 0} J_\Delta^i(t,\hbar) = \alpha_i A(X_-), i = III, IV, \tag{29}$$

where t belongs to the window (12). We note that the σ_i will depend on δ_1, δ_2 appearing in (12).

The intuition behind the result is the following. Choosing the positive numbers σ_1, σ_2, σ_3 small enough, and times t in the above window, the flow carries $\Omega_\sigma^{I,II}(\Delta)$ into a small neighborhood of X_+ and $\Omega_\sigma^{III,IV}(\Delta)$ into a neighborhood of X_-, as Δ tends to 0. More precisely, we shall prove that

$$\lim_{\Delta\to 0} \Phi_H^t(X) = X_+, \tag{30}$$

uniformly for all $X \in \Omega_\sigma^{I,II}(\Delta)$ and for all t in the window (12), and a similar statement for $\Omega_\sigma^{III,IV}(\Delta)$. This, together with the definition of the α_i (see (9)) and Proposition 3.7 clearly implies (29).

Assumption **(H2)** is a special case of **(H3)** (with $j = 0, +, -$), and it will be convenient for later reference in the proof of Theorem 2.3 to consider here assumption **(H3)** with its associated notations. We need to study classical paths starting from the small neighborhoods $\Omega_\sigma^i(\Delta) + X_j$ $(i = I, II, III, IV)$ of $X_j = (q_j, 0)$. We deal first with the case $i = II$. Let $\alpha \in [0, 1/2]$. Any point $X = (q,p)$ belonging to $\Omega_\sigma^{II}(\Delta) + X_j$ can then be labeled by a real x

$$q = q_j + xE^\alpha, \tag{31}$$

where $E = H(X) > 0$. We can therefore consider x and E as coordinates on $\Omega_\sigma^{II}(\Delta) + X_j$. Remark that clearly

$$|q - q_j| \le \Delta^{1-\sigma_3} \le H(X)^{\frac{1}{2}-\eta},\ \eta = \frac{\sigma_3 + \frac{\sigma_1}{2}}{1+\sigma_1}.$$

Consequently, if we choose $\alpha = \frac{1}{2} - \eta$, x belongs to $[-1, 1]$.

For simplicity of notation, we shall assume in the following $j \neq N_+$, but the case $j = N_+$ is treated in the same way.

We need an estimate on the time $\tau_E(\alpha, x)$ it takes to go from $(q_j, \sqrt{2E})$ to $(q = q_j + xE^\alpha, p = \sqrt{2(E - V(q_j + xE^\alpha))}$ along the curve $\{H = E\}$. A simple computation shows it satisfies, for any $\alpha \in [0, 1/2]$, when $E \searrow 0$,

$$\tau_E(\alpha, x) = |\int_{q_j}^{q_j + xE^\alpha} \frac{du}{\sqrt{2(E - V(u))}}| = \frac{1-2\alpha}{2\omega_j}|\log E| + O(1), \tag{32}$$

uniformly for x in a bounded set. In particular, if $\alpha = 0$, this shows that it takes a time

$$T_{j,j+1}(E) \equiv (\frac{1}{2\omega_j} + \frac{1}{2\omega_{j+1}})|\log E| + O(1)$$

to go from $(q_j, \sqrt{2E})$ to $(q_{j+1}, \sqrt{2E})$. Consequently, for every $\delta' > 0$, there exist σ_1, σ_2 such that, for all $\Delta^{2+\sigma_1} \leq E \leq \Delta^{2-\sigma_2}$,

$$T_\Delta^{(j)} + T_\Delta^{(j+1)} - \delta'|\log\Delta| \leq T_{j,j+1}(E) \leq T_\Delta^{(j)} + T_\Delta^{(j+1)} + \delta'|\log\Delta|. \tag{33}$$

On the other hand, if $\alpha = \frac{1}{2} - \eta$, we find

$$\tau_E(x,\alpha) = \frac{\eta}{\omega_j}|\log E| + O(1). \tag{34}$$

As a result, if $X = (q,p) \in \Omega_\sigma^{II}(\Delta) + X_j$ with $E = H(X)$ and x defined as in (31), then

$$\Phi_H^{T_{j,j+1}(E)}(X) = \Phi_H^{T_{j,j+1}(E)+\tau_E(x,\alpha)}(q_j, \sqrt{2E}) = \Phi_H^{\tau_E(x,\alpha)}(q_{j+1}, \sqrt{2E}).$$

Using now a normal form around X_{j+1} as in the proof of Lemma 3.4, together with (33) and (34), we easily conclude that, given $0 < \sigma_3' < 1$, there exist $0 < \sigma_1, \sigma_2, \sigma_3 < 1$ small enough so that

$$\Phi_H^{T_\Delta^{(j)}+T_\Delta^{(j+1)}}(\Omega_\sigma^{II}(\Delta) + X_j) \subset \Omega^{II}_{\sigma_1,\sigma_2,\sigma_3'}(\Delta) + X_{j+1}. \tag{35}$$

Now, for t in the window

$$(1+\delta_1)T_\Delta^{(j)} \leq t \leq T_\Delta^{(j)} + (2-\delta_2)T_\Delta^{(j+1)}, \tag{36}$$

we write $t = T_\Delta^{(j)} + T_\Delta^{(j+1)} + t'$ so that

$$-T_\Delta^{(j+1)} + \delta_1 T_\Delta^{(j)} \leq t' \leq (1-\delta_2)T_\Delta^{(j+1)}.$$

Hence, as in part (i), a direct application of the normal form around X_{j+1} shows that

$$\lim_{\Delta\to 0} \Phi_H^{t'}(X') = X_{j+1}, \quad \forall X' \in \Omega^{II}_{\sigma_1,\sigma_2,\sigma_3'}(\Delta) + X_{j+1},$$

provided σ_3' is small enough. Combining this with (35), we have finally proven that there exist $0 < \sigma_1, \sigma_2, \sigma_3 < 1$ so that, for all t in the window (36) and for all $X \in \Omega^{II}(\sigma)$, one has

$$\lim_{\Delta\to 0} \Phi_H^t(X) = X_{j+1}.$$

This, applied to $j = 0$, implies (30). For $\Omega^{IV}_{\sigma_1,\sigma_2,\sigma}(\Delta)$ the reasoning is completely analogous.

To treat the case where $i = I$, we introduce, for $E < 0$, $q_j^+(E)$ which is the (right) turning point, *i.e.* the smallest $q > q_j$ such that $V(q) = E$. Then $\tau_E(\alpha, x)$ denotes the time to go from $(q_j^+(E),0)$ to $(q=q_j^+(E)+x|E|^\alpha, p=\sqrt{2(E-V(q_j^+(E)+x|E|^\alpha)}$, $(x>0)$ along the curve $\{H=E\}$ and we have when $E\nearrow 0$

$$\tau_E(\alpha,x)=\int_{q_j^+(E)}^{q_j^+(E)+x|E|^\alpha}\frac{du}{\sqrt{2(E-V(u))}}=\frac{1-2\alpha}{2\omega_j}|\log(-E)|+O(1). \qquad (37)$$

The reasoning is then again similar as above and the case $i=III$ is treated analogously. ∎

Proof of Theorem 2.2: We have to estimate the integral

$$J_\Delta(t,\hbar)=(2\pi\hbar)^{-1}\iint_{\Omega_\sigma(\Delta)}A(\Phi_H^t(q,p))\rho\left(\frac{q}{\varepsilon},p\frac{\varepsilon}{\hbar}\right)dqdp, \qquad (38)$$

for $A\in C_0^\infty(\mathbb{R}^2)$ such that $\mathrm{supp}(A)\subset\{(q,p);\ q_-<q<q_+\}$. It is not difficult to see that we can always assume that A is supported in a small neighbourhood of one of the four branches of the zero-energy curve close to X_0.

In a first step we shall assume that the support of A is contained in $D_{\rho/2,0}$ for ρ small enough. We shall therefore be able to compute $J_\Delta(t,\hbar)$ using the normal form (Proposition 3.5). For simplicity we erase in what follows the index 0 ($F=F_0, f=f_0$). We will use the notation $J\approx M$ to mean that the difference $J-M$ is $O(\Delta^s)$ for some $s>0$. F is a symplectic transform so we get, after a slight modification of the σ's,

$$J_\Delta(t,\hbar)\approx(2\pi\hbar)^{-1}\iint_{\tilde\Omega_\sigma(\Delta)}\tilde A(\Phi_K^{t/f'(H\circ F^{-1}(\tilde X)}(\tilde q,\tilde p))\rho\left(\frac{q(\tilde X)}{\varepsilon},\,p(\tilde X)\frac{\varepsilon}{\hbar}\right)d\tilde q d\tilde p \qquad (39)$$

where $F^{-1}(\tilde X)=(q(\tilde X),p(\tilde X))$, $\tilde X=(\tilde q,\tilde p)$, $\tilde A=A\circ F^{-1}$ and

$$\tilde\Omega_\sigma(\Delta)=\{(q,p)\in\mathbb{R}^2,\Delta^{2+\sigma_2}\le|\tilde q\tilde p|\le\Delta^{2-\sigma_1},|\tilde q|+|\tilde p|\le\Delta^{1-\sigma_3}\}.$$

But $\tilde X$ is $\Delta^{1-\sigma_3}$-close to zero so it is not difficult to prove, applying Proposition 3.5, that we are allowed to linearize F^{-1} so that we have

$$F^{-1}(\tilde X)=\frac{1}{\sqrt2}(\tilde q+\omega_0\tilde p,-\frac{\tilde q}{\omega_0}+\tilde p)+O(|\tilde X|^2).$$

We also have $f'(H\circ F^{-1}(\tilde X))=f'(0)+O(|\tilde X|)$. So we get, using the explicit expression for the flow of the Hamiltonian K, $J_\Delta(t,\hbar)\approx J_\Delta^0(t,\hbar)$, where

$$\begin{aligned}J_\Delta^0(t,\hbar)=\frac{1}{2\pi\hbar}&\iint_{\tilde\Omega_\sigma(\Delta)}\tilde A(\mathrm{e}^{t\omega_0}\tilde q,\mathrm{e}^{-t\omega_0}\tilde p)\\&\times\rho\left(\frac{1}{\sqrt2\varepsilon}(\tilde q+\omega_0\tilde p),\,(-\frac{\tilde q}{\omega_0}+\tilde p)\frac{\varepsilon}{\sqrt2\hbar}\right)d\tilde q d\tilde p.\end{aligned} \qquad (40)$$

Now the result of the computation of the limit for Δ going to 0 of the last integral depends on the relative size of ε and $\hbar$. There are three different cases to check: $\varepsilon\approx\sqrt\hbar$, $\varepsilon=o(\sqrt\hbar)$, $\sqrt\hbar=o(\varepsilon)$.

Let us begin with the symmetric case when $\lim_{\varepsilon\to 0}\dfrac{\hbar}{\varepsilon^2} = c$, $0 < c < +\infty$. Now we compute the limit with the change of variables: $\tilde q = \mathrm{e}^{-t\omega_0}u$, $\tilde p = \mathrm{e}^{-t\omega_0}v\frac{\hbar}{\varepsilon^2}$ and obtain under the extra condition $\lim_{\varepsilon\to 0}\varepsilon \mathrm{e}^{t\omega_0} = \kappa$:

$$\begin{aligned}\lim_{\Delta\to 0} J^0_\Delta(t,\hbar) &= \frac{1}{2\pi\kappa^2}\iint_{\mathbb{R}^2}\tilde A(u,0)\rho\left(\frac{1}{\sqrt{2}\kappa}(u+c\omega_0 v), \frac{1}{\sqrt{2}\kappa}(v-\frac{u}{c\omega_0}\right) dudv\\ &= \int_{\mathbb{R}}\tilde A(u,0)G_{\kappa,c,2}(u)du,\end{aligned}$$

where we used (14). Let us remark that close to zero, in the phase space, we have $\{\tilde p = 0\}$ if and only if $\{p = p(q) = \pm\sqrt{-2V(q)}\}$ where $\pm = +$ if $q > 0$ and $\pm = -$ if $q < 0$. So to come back to the curve Σ_0, let us try to compute the right hand side with the change of variable $u = \tilde q(q,p(q))$. For that purpose, we compute $\frac{d\tilde q}{dq}(q,p(q)) = \frac{\partial\tilde q}{\partial q} + p'(q)\frac{\partial\tilde q}{\partial p}$. By taking the first X-derivative in the normal form expression we have

$$f'(H(X))H'(X) = F'(X)^* K'(F(X)) \tag{41}$$

where M^* denotes the transpose of the matrix M. So we get ($f'(0) = \omega_0^{-1}$)

$$\begin{pmatrix} V'(q)\\ p\end{pmatrix} = \omega_0\begin{pmatrix}\frac{\partial\tilde q}{\partial q} & \frac{\partial\tilde p}{\partial q}\\ \frac{\partial\tilde q}{\partial p} & \frac{\partial\tilde p}{\partial p}\end{pmatrix}\begin{pmatrix}\tilde p\\ \tilde q\end{pmatrix} \tag{42}$$

A little algebraic computation gives

$$\frac{d\tilde q}{dq}(q,p(q)) = \pm\frac{\omega_0}{\sqrt{-2V(q)}}\tilde q, \tag{43}$$

leading to

$$\tilde q = \exp\left(\pm\omega_0\int_{q_0}^{q}\frac{du}{\sqrt{-2V(u)}}\right)\tilde{q}_0. \tag{44}$$

We shall compute $\tilde q(q,p(q))$ more explicitly by going to the limit $q_0 \to 0$. We can easily compute $\frac{d\tilde q}{dq}(0,0)$; hence using the Taylor formula we have

$$\tilde{q_0} = \frac{1}{\sqrt{2}}q_0 + O(q_0^2) \tag{45}$$

so that

$$\tilde q = \frac{1}{\sqrt{2}}|q|\exp\left(\pm\int_0^q\left(\frac{\omega_0}{\sqrt{-2V(u)}} - \frac{1}{u}\right)du\right) \equiv \ell(q). \tag{46}$$

This finally yields

$$\lim_{\Delta\to 0} J^0_\Delta(t,\hbar) = \omega_0\int_{q_-}^{q_+} A(q,p(q))\ell(q)G_{\kappa,c,2}(\ell(q))\frac{dq}{\sqrt{-2V(q)}}. \tag{47}$$

This proves Theorem 2.2 in the symmetric case $\epsilon^2 \sim \hbar$ when A is supported in a small neighborhood of 0. For the two other cases the computation is almost the same and is left to the reader.

Let us now assume that A is supported outside a small disc $D_{\rho/4,0}$. The general case will follow using a partition of unity. It is enough to assume that A is supported in $\{(q,p);\ p \geq 0,\ q_- + \delta < q < q_+ - \delta, \Delta^{2+\sigma_1} \leq |H(q,p)| \leq \Delta^{2-\sigma_2}\}$, for some $\delta > 0$ and $\sigma_j > 0$. By the same argument already used in the proof of Theorem 2.1 (ii), there exists a finite time $T_1 > 0$ depending only on δ such that $A \circ \Phi_H^{T_1}$ is supported in $D_{\rho/2,0}$. So we can apply the result proved in the first step to $A_1 := A \circ \Phi_H^{T_1}$. More explicitely we have

$$J_\Delta(t,\hbar) = (2\pi\hbar)^{-1} \iint_{\Omega_\sigma(\Delta)} A_1(\Phi_H^{t+T_1}(q,p))\rho\left(\frac{q}{\varepsilon}, p\frac{\varepsilon}{\hbar}\right) dqdp, \tag{48}$$

So we get, for a new constant $\kappa_1 := \mathrm{e}^{\omega_0 T_1}\kappa$,

$$\lim_{\Delta\to 0} J_\Delta(t,\hbar) = \int_{\Sigma_{unst}} A_1(X) g_{\kappa_1,c,\mu}(X) d\Sigma_0(X). \tag{49}$$

To get an invariant formula we parametrize the curve Σ_0 with the time of the classical flow (this is possible because A is supported outside the equilibrium points. Then we translate in time by T_1 and remark that an explicit computation gives easily $\ell(q_{s+T_1}) = \mathrm{e}^{\omega_0 T_1}\ell(q_s)$. Hence we get finally

$$\int_{\Sigma_{\mathrm{unst}}} A_1(X) g_{\kappa_1,c,\mu}(X) d\Sigma_0(X) = \int_{\Sigma_{\mathrm{unst}}} A(X) g_{\kappa,c,\mu}(X) d\Sigma_0(X), \tag{50}$$

which is the expected formula to end the proof of Theorem 2.2. ∎

Proof of Theorem 2.3: This Theorem is an extension of Theorem 2.1 (ii). We obtain the proof in this more general case easily from the proof of Theorem 2.1 (ii) where the general mechanism for multiple wells has already been described. We only sketch the argument leading to (16) and (17).

Fix $0 < \ell \leq N_+$. Remembering that $T_\Delta^{(j)} = T_\Delta^{(0)}$ in this case and iterating equation (35) ℓ times, one proves easily that, given $0 < \sigma_3' < 1$, there exist $0 < \sigma_1, \sigma_2, \sigma_3 <$ small enough, so that

$$\Phi_H^{2\ell T_\Delta^{(0)}}(\Omega_\sigma^{II}(\Delta)) \subset \Omega_{\sigma_1,\sigma_2,\sigma'}^{II}(\Delta) + X_\ell.$$

¿From this one concludes as before that there exist $0 < \sigma_1, \sigma_2, \sigma_3 <$ so that for all $X \in \Omega_\sigma^{II}(\Delta)$,

$$\lim_{\Delta\to 0} \Phi_H^t(X) = X_\ell,$$

for all t such that

$$(2\ell - 1 + \delta_1)T_\Delta^{(0)} \leq t \leq (2\ell + 1 - \delta_2)T_\Delta^{(0)}.$$

This in turn implies as before that, for such t,

$$\lim_{\Delta\to 0} J_\Delta^{II}(t,\hbar) = \alpha_{II} A(X_\ell).$$

Similarly,

$$\lim_{\Delta\to 0} J^{IV}_{\Delta}(t,\hbar) = \alpha_{IV} A(X_{-\ell}).$$

For the component Ω^I, one has to remark that a trajectory $\Phi^t_H(X)$, with $X \in \Omega^I_\sigma(\Delta)$ will, after visiting X_+ for t between $(1+\delta_1)T^{(0)}_\Delta$ and $(3-\delta_2)T^{(0)}_\Delta$, return to a neighbourhood of X_0 during the period $[(3+\delta_1)T^{(0)}_\Delta, (5-\delta_2)T^{(0)}_\Delta]$ *etc.*. This explains the difference between (16) and (17). ∎

Proof of Theorem 2.4: This is an easy consequence of the preceding arguments, where one has to follow the four components of the initial Wigner function separately in their journey from one X_j to another.

Indeed, this time, a trajectory $X \in \Omega^{II}_\sigma(\Delta)$, will be close to X_1 for t between $T^{(0)}_\Delta + \delta_1|\log\Delta|$ and $T^{(0)}_\Delta + 2T^{(1)}_\Delta - \delta_2|\log\Delta|$, then it will be close to X_2 for t between $T^{(0)}_\Delta + 2T^{(1)}_\Delta + \delta_1|\log\Delta|$ and $T^{(0)}_\Delta + 2T^{(1)}_\Delta + 2T^{(2)}_\Delta - \delta_2|\log\Delta|$, *etc.*. A similar statement holds for $X \in \Omega^i_\sigma(\Delta)$, with $i = I, III, IV$, but contrary to what happens in the previous theorem, with different time-intervals. Taking the intersection of the intervals where the dynamics is controlled yields the set I of the statement of the theorem. ∎

References

[BB] Berry, M. V., Balasz N.L., *Evolution of semi-classical quantum states in phase space*, J. Phys. A **12**, 625-642 (1979)

[BGP] D. Bambusi, S. Graffi S., T. Paul, *Long time semi-classical approximation of quantum flows: a proof of the Ehrenfest time*, Asymptot. Anal. 21 (1999), no. 2, 149–160.

[BDB1] F. Bonechi, S. De Bièvre, *Exponential mixing and* $\ln\hbar$ *time scales in quantized hyperbolic maps on the torus,* mp_arc 99-381 (1999), Comm. Math. Phys. **211** 3, 659-686 (2000).

[BDB2] F. Bonechi, S. De Bièvre, *Controlling strong scarring for quantized ergodic toral automorphisms*, mp_arc 02-81(2002), Duke Math. Journal, to appear.

[BR] A. Bouzouina, D. Robert. *Uniform semi-classical estimates for the propagation of quantum observables,* Duke Math. Journal (to appear).

[CP1] Y. Colin de Verdière, B. Parisse. *Équilibre instable en régime semi-classique : I-Concentration microlocale,* Comm. Partial Differential Equations, 19 (9&10), 1535-1563 (1994).

[CP2] Y. Colin de Verdière, B. Parisse. *Singular Bohr-Sommerfeld Rules,* Comm. Math. Phys. 205, 459-500 (1999).

[CC] Casati, G., Chirikov, B., The legacy of chaos in quantum mechanics, in "Quantum Chaos", Ed. G. Casati and B. Chirikov, Cambridge University Press (1995).

[CV] Y. Colin de Verdière, J. Vey, *Le lemme de Morse isochore,* Topology, vol. 18, 283-293 (1979).

[CR] M. Combescure M., D. Robert. *Semi-classical spreading of quantum wave packets and applications near unstable fixed point of the classical flow*, Note CRAS Paris, t.323, Série I, pp. 871-876 (1996) and Asymptotic Analysis 14, pp. 377-404 (1997).

[DR] M. Dauge, D. Robert, *Weyl's formula for a class of pseudodifferential operators with negative order on* $L^2(\mathbb{R}^n)$*,* Lecture Notes in Math. No. 1259, 90-122, Springer-Verlag (1986).

[DB] S. De Bièvre, *Chaos, quantization and the classical limit on the torus*, "Proceedings of the XIVth workshop on geometric methods in physics, Bialowieza July 1995" – Polish Scientific Publishers PWN (1998).

[F] G.B. Folland , *Harmonic Analysis in Phase Space.* Annals of Math. Studies, 122, Princeton University Press (1989).

[HJ] G. Hagedorn , A. Joye, *Exponentially Accurate Semi-classical Dynamics: Propagation, Localization, Ehrenfest Times, Scattering, and More General States*, Ann. Henri Poincaré **1**, no. 5, 837–883 (2000).

[HS] B. Helffer, J. Sjöstrand, *Semi-classical analysis for Harper's equation III,* Bull. Soc. Math. France 117 (4) mémoire No 39 (1989).

[OTH] O'Connor, P.W. , Tomsovic, S., Heller, E.J., *Semi-classical dynamics in the strongly chaotic regime: breaking the log time barrier*, Physica **55** D, 340-357 (1992).

[R] D. Robert, *Autour de l' Approximation Semi-classique*, **PM 68**, Birkhäuser, 1987.

[TH] Tomsovic, S. , Heller, E.J., *Semi-classical dynamics of chaotic motion: unexpected long-time accuracy*, Phys. Rev. Lett. **67** 6, 664 (1991).

[T] J.Toth, *On the small-scale mass concentration of modes* Comm. Math. Phys. 206, 409-428 (1999).