

A Probabilistic Approach to Semi-classical Approximations

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We study in this paper the semi-classical expansion of the Schrödinger equation, using a probabilistic approach based on the Wiener measure. Using almost-analytic extensions, we exhibit a probabilistic ansatz for the wave function. We show that this ansatz approximates very well the wave function in the semi-classical regime, and gives the semi-classical expansion under mild hypothesis on the potential at infinity, and no analyticity conditions. In this paper, the study takes place before the caustics. © 1996 Academic Press, Inc.

1. INTRODUCTION

We give in this paper a new probabilistic approach to the semi-classical approximation of the Schrödinger equation, i.e. the behavior when the Planck's constant h tends to zero, of the solution $\Phi(t, x)$ of

$$\begin{cases} i\hbar \frac{\partial \Phi}{\partial t} + \frac{\hbar^2}{2} \Delta \Phi - V\Phi = 0 \\ \Phi(0, x) = f(x) e^{(i/\hbar) s(x)} \end{cases}$$

where f, s, V are smooth functions.

This is indeed an old question, and with no claim of completeness, we can quote the following references in the physics literature, starting from

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Van Vleck ('28) [23], Feynman ('45) [10], Voros [24], and two recent surveys in the books of Schulman [20] and Gützwiler [13].

In the mathematical literature, one can distinguish two different approaches. The first one, for which a good source could be the books of Guillemin & Sternberg [12], and of Robert [19], is purely analytical. This approach is very complete and efficient, but very far from the physical picture given by the path integral formalism. The second one tries to stay closer to this physical intuition and is probabilistic in nature. One can distinguish there two different lines of attack: the first one is to build rigorously a Feynman integration, and has been pursued by Albeverio & Hoegh-Krohn [3], Elworthy & Truman [9], Kallianpur, Kannan & Karandikar [15], and more recently by Albeverio & Brzeźniak [2]. The intrinsic limitation of the scope of these results seems to be on the class of potentials V that can be handled, i.e. V should be a quadratic form, plus the Fourier transform of a signed measure. This very global hypothesis is necessary for the rigorous Feynman integral formalism developed by Albeverio & Hoegh-Krohn.

The second line is to extend analytically the Feynman–Kac formula for solutions of the heat equation. The general opinion about this very appealing strategy is resumed by Berezin & Shubin [7] when they say that “it runs into practically insurmountable difficulties”. We want here to show that this strategy based on Wiener measure, can indeed be implemented for general smooth potentials. It must be noticed that if one is ready to assume very strong analyticity hypothesis on the potentials, this strategy has been successfully used by Doss [8], and by Azencott & Doss [5]. Our trick to avoid these analyticity assumptions is to use the almost-analytic machinery introduced by Melin & Sjöstrand [18], to complexify the Feynman–Kac formula. This almost-analytic extension of the Feynman–Kac formula does not give an exact probabilistic representation of the wave function, but it enables us to give a probabilistic ansatz which, although it does not solve the Schrödinger equation, gives a very good approximation of its solution; and to which the available stationary phase results on Wiener space proved in [6], can be applied to get semi-classical expansions in any Sobolev norm, or uniform norm.

The error between the ansatz and the true solution is of order $O(\hbar^\infty)$ in L^2 -norm with no assumption on V , except smoothness and essential self-adjointness of the operator $-\hbar^2/2 \Delta + V$. To get estimates in better norms is a purely analytical problem. We propose some results in H^1 -norm, and uniform norm, which are certainly not optimal. But it should be noticed that our ansatz gives the semi-classical approximation in a given norm as soon as the problem is “semi-classically localizable” in this norm, which is a necessary condition for the expansion to be valid (see the discussion of Section 4.4).

Our discussion is for this paper, limited to the short time problem, i.e. before caustics. We expect to extend this approach after caustics in a forthcoming paper.

2. A PROBABILISTIC ANSATZ USING ALMOST-ANALYTIC EXTENSIONS

The following assumptions will be made throughout the paper.

- H1. f, V, s are \mathcal{C}^∞ from \mathbb{R}^d to \mathbb{R} .
- H2. f has compact support K in \mathbb{R}^d .
- H3. The classical motion defined by V is complete.

Assumption H3 is not essential. It simply avoids to consider explosion times for the classical trajectories. But it is easy to see that all our results will be true if we remove H3, and if we limit the study before these explosion times.

2.1. Description of the Probabilistic Ansatz

For each $t > 0$, and each $x \in \mathbb{R}^d$, let us consider the classical mechanics system

$$\begin{cases} \ddot{\gamma}_s + \nabla V(\gamma_s) = 0, & \forall s \leq t \\ \gamma_0 = x \\ \dot{\gamma}_t + \nabla s(\gamma_t) = 0 \end{cases} \quad (\mathcal{C}_t^x)$$

where ∇V and ∇s stand for the gradient of the functions V and s , and γ is a continuous path from $[0, t]$ to \mathbb{R}^d .

PROPOSITION 2.1. *Let V be a smooth potential from \mathbb{R}^d to \mathbb{R} , such that the classical motion associated to V is complete. Let K be a compact set in \mathbb{R}^d . $K_t = \{x \in \mathbb{R}^d, (\mathcal{C}_t^x) \text{ has a solution ending at time } t \text{ in } K\}$ is a compact set of \mathbb{R}^d . Moreover, there exists $T_K > 0$ such that for all $t < T_K$, for all x in some open neighborhood O_t of K_t , (\mathcal{C}_t^x) has a unique solution $\gamma_t^x(s)$. This solution is \mathcal{C}^∞ in x , \mathcal{C}^1 in t , and ends in K (i.e. $\gamma_t^x(t) \in K$), whenever $x \in K_t$.*

Though classical, we give the proof of Proposition 2.1 in Appendix 1.

Let $\tilde{f}, \tilde{V}, \tilde{s}$ be some almost-analytic continuations of f, V, s . Thus $\tilde{f}, \tilde{V}, \tilde{s}$ are \mathcal{C}^∞ functions from \mathbb{C}^d to \mathbb{C} satisfying

- $\tilde{V}|_{\mathbb{R}^d} = V, \tilde{f}|_{\mathbb{R}^d} = f, \tilde{s}|_{\mathbb{R}^d} = s;$
- $\forall K$ compact of $\mathbb{R}^d, \forall k \in \mathbb{N}, \forall \alpha, \beta \in \mathbb{N}^d$ such that $|\beta| = \sum_{i=1}^d \beta_i \geq 1,$
 $\exists C > 0,$ such that $\forall x \in K, \forall y \in \mathbb{R}^d,$

$$|D_{(\alpha, \beta)} \tilde{f}(x + iy)| \leq C |y|^k$$

$$|D_{(\alpha, \beta)} \tilde{V}(x + iy)| \leq C |y|^k$$

$$|D_{(\alpha, \beta)} \tilde{s}(x + iy)| \leq C |y|^k$$

where $D_{(\alpha, \beta)} = \partial^{|\alpha| + |\beta|} / (\partial z_1^{\alpha_1} \dots \partial z_d^{\alpha_d} \partial \bar{z}_1^{\beta_1} \dots \partial \bar{z}_d^{\beta_d})$, $z_k = x_k + iy_k$.

The reader is referred to [22] for the definition, existence and elementary properties of almost-analytic continuations. We just want to underline that almost-analytic continuations are not unique. Two almost-analytic continuations differ one from the other by a smooth function, which is flat on the real axis (i.e. in x), but whose behavior in y near ∞ is free. For this reason, it can be assumed that $\tilde{f}, \tilde{s}, \tilde{V}$ are null for $|y| \geq r$, for some $r > 0$. Moreover, since f has compact support, \tilde{f} can be taken with compact support in \mathbb{C}^d .

From now on, the same notations will be used for f, s, V and their almost-analytic continuations. Moreover, ε^2 will denote \hbar . Using these almost-analytic extensions, we guess that the function $\Psi(t, x)$ defined (whenever it is possible) by

$$\Psi(t, x) = E \left[f(\gamma_t^x(t) + \sqrt{i\varepsilon}B_t) \exp \left(-\frac{H(t, x, \varepsilon B)}{\varepsilon^2} \right) \right] \tag{2}$$

where H is defined by

$$\begin{aligned} H(t, x, \varepsilon B) = & -is(\gamma_t^x(t) + \sqrt{i\varepsilon}B_t) + i \int_0^t V(\gamma_t^x(s) + \sqrt{i\varepsilon}B_s) ds \\ & + \frac{1}{\sqrt{i}} \int_0^t \dot{\gamma}_t^x(s) \delta(\varepsilon B_s) - \frac{i}{2} \int_0^t |\dot{\gamma}_t^x(s)|^2 ds \end{aligned} \tag{3}$$

should be a good approximation of the solution to Schrödinger equation. Before explaining to what extent this assertion is true, we would like to tell where this ansatz comes from.

Under analyticity assumptions for s, f, V , and additional assumptions for which we refer the reader to [8], H. Doss has proved in [8] that

$$E \left[(f e^{is/\varepsilon^2})(x + \sqrt{i\varepsilon}B_t) \exp \left(\frac{-i}{\varepsilon^2} \int_0^t V(x + \sqrt{i\varepsilon}B_s) ds \right) \right] \tag{4}$$

is a solution of the Schrödinger equation.

Extending analytically the Cameron–Martin formula, R. Azencott & H. Doss ([5]) have shown that (4) is equal to (2), which is the natural expression to obtain semi-classical approximations.

In our context, where the analyticity assumptions are removed, the analytical extension of Cameron–Martin formula is no longer valid, so that (2) and (4) are no longer equal. Our goal being here to obtain semi-classical expansions, we have chosen to work directly on (2).

2.2. Equation Satisfied by the Probabilistic Ansatz

PROPOSITION 2.2. 1. $\exists T^r > 0$ such that Ψ can be defined on $[0, T^r] \times \mathbb{R}^d$, and is $\mathcal{C}^{1, \infty}$ on this space (that is \mathcal{C}^1 in t , and \mathcal{C}^∞ in x). For all $t < T^r$, $\Psi(t, \cdot)$ has compact support in K_t^r .

2. Ψ satisfies the equation

$$\forall t < T^r, \quad i \frac{\partial \Psi}{\partial t} + \frac{\varepsilon^2}{2} \Delta \Psi - \frac{V}{\varepsilon^2} \Psi = E[Z(t, x, \varepsilon, \varepsilon B) \exp^{-(1/\varepsilon^2) H(t, x, \varepsilon B)}] \quad (5)$$

where

(a) H is defined by (3), and

$$(b) \quad Z(t, x, \varepsilon, \varepsilon B) = \sum_{j=-1, 0, 1} \varepsilon^{2j} Z_j(t, x, \varepsilon B). \quad (6)$$

$Z_j(t, \cdot, \omega)$ has compact support in K_t^r , and satisfies $\forall k \in \mathbb{N}, \exists C > 0$, such that $\forall t < T^r$,

$$\sup_{s \leq t} \sup_{x \in \mathbb{R}^d} |Z_j(s, x, \omega)| \leq C \|\omega\|_t^k, \quad a.s \quad (7)$$

where $\|\omega\|_t$ denotes the uniform norm in $\mathcal{C}([0, t], \mathbb{R}^d)$.

3. When the functions f, s, V , are analytic on a strip around the real axis, then $\exists r_0 > 0$ such that $Z_j(t, x, \omega) \mathbb{1}_{\|\omega\|_t \leq r_0} = 0$ a.e.

Remark 2.3. Using property (7), one can therefore expect $E(Ze^{-H/\varepsilon^2})$ to be $O(\varepsilon^k)$ for all k , i.e. the remainder term to be “small”. This is actually the case, and will be proved in Section 4.

Proof of Proposition 2.2.

Proof of Proposition 2.2.1. We first prove that ψ is well defined, at least for small times. Let \tilde{K} be the (compact) support of f in $\mathbb{C}^d \sim \mathbb{R}^{2d}$. Then \tilde{K} is a subset of $\{x + iy, x \in K, |y| \leq r\}$. Let us define

$$K^r = \{x \in \mathbb{R}^d, \exists \tilde{x} \in K, |x - \tilde{x}| \leq r\}$$

K^r is a compact set in \mathbb{R}^d , and we associate to K^r the time T^r , and the sets K_t^r and O_t^r , in the same way as in Proposition 2.1, the time T_K and the sets K_t and O_t were associated to K . Whenever $\gamma_t^x(t) \notin K^r$, $\Psi(t, x) = 0$.

Therefore, the support of $\Psi(t, \cdot)$ is included in K_t^r . Moreover, for all $t < T^r$ and all $x \in K_t^r$,

$$\left| f(\gamma_t^x(t) + \sqrt{i\varepsilon}B_t) \exp \left(+\frac{i}{\varepsilon^2} s(\gamma_t^x(t) + \sqrt{i\varepsilon}B_t) - \frac{i}{\varepsilon^2} \int_0^t V(\gamma_t^x(s) + \sqrt{i\varepsilon}B_s) ds \right) \right|$$

$$\leq \|f\|_{\bar{K}} \exp \left(\frac{1}{\varepsilon^2} \|\Im m s\|_{\bar{K}} \right) \exp \left(\frac{t}{\varepsilon^2} \sup_{\substack{|y| \leq \sqrt{2}r \\ x \in \cup_{s \leq t} K_s^r}} |\Im m V(x + \sqrt{i}y)| \right)$$

where $\|f\|_{\bar{K}} = \sup_{z \in \bar{K}} |f(z)|$.

But, when $t < +\infty$, $\cup_{s \leq t} K_s^r$ is compact. Therefore,

$$f(\gamma_t^x(t) + \sqrt{i\varepsilon}B_t) \exp \left(-\frac{1}{i\varepsilon^2} s(\gamma_t^x(t) + \sqrt{i\varepsilon}B_t) + \frac{1}{i\varepsilon^2} \int_0^t V(\gamma_t^x(s) + \sqrt{i\varepsilon}B_s) ds \right)$$

is bounded, and expression (2) makes sense for all $t < T^r$, and all $x \in \mathbb{R}^d$ (when $x \notin K_t^r$, (2) is taken equal to 0).

Let us now study the differentiability of Ψ . Let X_H denote the Hamiltonian vector field associated to V ,

$$X_H: \mathbb{R}^d \times \mathbb{R}^d \rightarrow \mathbb{R}^d \times \mathbb{R}^d$$

$$(q, p) \mapsto (p, -\nabla V(q))$$

Let $\phi_s(q, p)$ denote the Hamiltonian flow, that is the flow of diffeomorphisms of \mathbb{R}^{2d} associated to X_H , and π denote the first projection π :

$$\mathbb{R}^d \times \mathbb{R}^d \rightarrow \mathbb{R}^d.$$

$$(q, p) \mapsto q.$$

Let us define $\varphi_t(q, p) = \pi \circ \phi_t(q, p)$, and

$$G(t, q, p) = E \left[F(\varphi(q, p) + \sqrt{i\varepsilon}B) \exp \left(-\frac{1}{\sqrt{i\varepsilon}} \int_0^t \dot{\varphi}_s(q, p) \delta B_s - \frac{1}{2i\varepsilon^2} \int_0^t |\dot{\varphi}_s(q, p)|^2 ds \right) \right] \tag{8}$$

where for all continuous path ω from $[0, t]$ to \mathbb{C}^d ,

$$F(\omega) = f(\omega_t) \exp \left(\frac{i}{\varepsilon^2} s(\omega_t) - \frac{i}{\varepsilon^2} \int_0^t V(\omega_s) ds \right). \tag{9}$$

Then $\Psi(t, x) = G(t, x, \dot{\gamma}_t^x(0))$. The differentiability of G in t is an easy consequence of Itô formula. The differentiability of G in (q, p) follows from the

differentiability of ϕ and its derivatives in (q, p) , and from the smoothness of the coefficients f, s, V . Proposition 2.1 enables us to conclude that before the caustics, Ψ is $\mathcal{C}^{1, \infty}$.

Proof of Proposition 2.2.2. Before computing $i(\partial\Psi/\partial t) + (\varepsilon^2/2) \Delta\Psi - (V/\varepsilon^2)\Psi$, we introduce some notations.

- $\forall z \in \mathbb{C}^d, |z|_c^2 = |\Re z|^2 - |\Im z|^2 + 2i(\Re z, \Im z)$,
- $\mathcal{W}_t = \{\text{continuous paths from } [0, t] \text{ to } \mathbb{R}^d\}$,
- $\mathcal{W}_t(\mathbb{C}) = \{\text{continuous paths from } [0, t] \text{ to } \mathbb{C}^d\}$.

\mathcal{W}_t and $\mathcal{W}_t(\mathbb{C})$ are endowed with the uniform convergence topology, denoted by $\|\cdot\|_t$.

Denote for every function $F: \mathcal{W}_t(\mathbb{C}) \rightarrow \mathbb{R}$ Fréchet differentiable (with derivative dF), for all $\omega \in \mathcal{W}_t(\mathbb{C})$, and all $h \in \mathcal{W}_t$,

$$D_r F(\omega) h = dF(\omega) \cdot h, \quad D_i F(\omega) h = dF(\omega) \cdot (ih)$$

$$DF = \frac{1}{2}(D_r F - iD_i F), \quad \bar{D}F = \frac{1}{2}(D_r F + iD_i F).$$

Finally, let Θ be a bounded domain in \mathbb{R}^n , and $(g_s(\theta), s \leq t)$ a path in $\mathcal{W}_t(\mathbb{C})$, depending smoothly on $\theta \in \Theta$. We define for all $k \in \mathbb{N}$ and all $p > 1$, the space

$$\mathcal{D}_{p,k}^g(\Theta) = \left\{ F: \mathcal{W}_t(\mathbb{C}) \mapsto \mathbb{R}, k\text{-times Fréchet differentiable, such that} \right.$$

$$\left. \sum_{l \leq k} \sup_{\theta \in \Theta} \|d^{(l)}F(g(\theta) + \sqrt{i\varepsilon}B)\|_{HS} \|L_p\| < +\infty \right\}$$

where $\|\cdot\|_{HS}$ denotes the Hilbert–Schmidt norm.

We have then the following lemma:

LEMMA 2.4. *Let $(g_s(\theta), s \leq t)$ a path in $\mathcal{W}_t(\mathbb{C})$, depending smoothly on $\theta \in \Theta$, and 2-times continuously differentiable in s . Assume that F is in $\mathcal{D}_{p,k}^g(\Theta)$ for some $k \geq 2$, and some $p > 1$. Let us define*

$$G(t, \theta) = E \left[F(g(\theta) + \sqrt{i\varepsilon}B) \exp \left(-\frac{1}{\sqrt{i\varepsilon}} \int_0^t \dot{g}_s(\theta) \delta B_s - \frac{1}{2i\varepsilon^2} \int_0^t |\dot{g}_s(\theta)|_c^2 ds \right) \right].$$

Then G is $(k - 1)$ -differentiable in Θ , and $\forall j \in \{1, \dots, n\}, \forall \theta \in \Theta$,

$$\frac{\partial G}{\partial \theta_j}(t, \theta) = E \left[\left(D_r F \cdot \frac{\partial g_0^r}{\partial \theta_j} + D_i F \cdot \frac{\partial g_0^i}{\partial \theta_j} + (1 + i) \bar{D}F \cdot \left(\frac{\partial g^r}{\partial \theta_j} - \frac{\partial g^r}{\partial \theta_j} - \frac{\partial g^i}{\partial \theta_j} + \frac{\partial g^i}{\partial \theta_j} \right) \right) \right.$$

$$\left. \times \exp \left(-\frac{1}{\sqrt{i\varepsilon}} \int_0^t \dot{g}_s \delta B_s - \frac{1}{2i\varepsilon^2} \int_0^t |\dot{g}_s|_c^2 ds \right) \right] \tag{11}$$

where

1. the derivatives of F are evaluated at $g(\theta) + \sqrt{i\varepsilon}B$;
2. g and its derivatives are evaluated at θ ;
3. $\partial g_0^l / \partial \theta_j$ ($l=r, i$) denotes the constant path in $\mathbb{R}^d: s \mapsto \partial g_0^l / \partial \theta_j$.

The reader is referred to Appendix 2 for the proof of Lemma 2.4. From Lemma 2.4, we get

LEMMA 2.5.

$$i \frac{\partial \Psi}{\partial t} + \frac{\varepsilon^2}{2} \Delta \Psi - \frac{V}{\varepsilon^2} \Psi = i \frac{\partial G}{\partial t} + \frac{\varepsilon^2}{2} \Delta_q G - \frac{V}{\varepsilon^2} G + E \left[Z \exp \left(-\frac{H}{\varepsilon^2} \right) \right] \quad (12)$$

where Z satisfies (6) and (7), and G is defined by (8).

Proof of Lemma 2.5. A simple computation yields

$$\begin{aligned} & i \frac{\partial \Psi}{\partial t} + \frac{\varepsilon^2}{2} \Delta \Psi - \frac{V}{\varepsilon^2} \Psi \\ &= i \frac{\partial G}{\partial t} + \frac{\varepsilon^2}{2} \Delta_q G - \frac{V}{\varepsilon^2} G + \frac{\varepsilon^2}{2} \frac{\partial G}{\partial p} \Delta_x \dot{\gamma}_t^x(0) + i \frac{\partial G}{\partial p} \cdot \frac{\partial \dot{\gamma}_t^x(0)}{\partial t} \\ & \quad + \varepsilon^2 \text{Trace} \left(\frac{\partial^2 G}{\partial q \partial p} \frac{\partial \dot{\gamma}_t^x(0)}{\partial x} \right) + \frac{\varepsilon^2}{2} \text{Trace} \left(\frac{\partial^2 G}{\partial p^2} \frac{\partial \dot{\gamma}_t^x(0)}{\partial x} \left(\frac{\partial \dot{\gamma}_t^x(0)}{\partial x} \right)' \right) \end{aligned}$$

where

$$\begin{aligned} \frac{\partial^2 G}{\partial q \partial p} &= \left(\frac{\partial^2 G}{\partial q_i \partial p_j} \right)_{i,j}, & \frac{\partial^2 G}{\partial p^2} &= \left(\frac{\partial^2 G}{\partial p_i \partial p_j} \right)_{i,j}, \\ \Delta_q G &= \sum_{i=1}^d \frac{\partial^2 G}{\partial q_i^2}, & \frac{\partial G}{\partial p} &= \left(\frac{\partial G}{\partial p_j} \right)_j, \\ \frac{\partial \dot{\gamma}_t^x(0)}{\partial x} &= \left(\frac{\partial \dot{\gamma}_t^x, i(0)}{\partial x_j} \right)_{i,j}, & \Delta_x \dot{\gamma}_t^x(0) &= \sum_{i=1}^d \frac{\partial^2 \dot{\gamma}_t^x(0)}{\partial x_i^2}. \end{aligned}$$

In order to compute $\partial G / \partial p$, let us apply Lemma 2.4 with $n = 2d$, $\theta = (q, p)$, F defined by (9), and the real path $g(\theta) = \varphi(q, p)$. It is clear that F is in all the spaces $\mathcal{D}_{p,k}^\varphi(\mathcal{O}_r)$ (remember that $f(\varphi_u + \sqrt{i\varepsilon}B_u)$, $s(\varphi_u + \sqrt{i\varepsilon}B_u)$, $V(\varphi_u + \sqrt{i\varepsilon}B_u)$ are null whenever $|\varepsilon B_u| \geq \sqrt{2}r$). Since $\varphi_0(q, p) = q$, (11) leads to

$$\frac{\partial G}{\partial p_j}(t, x, \dot{\gamma}_t^x(0)) = E \left[\exp \left(-\frac{1}{\varepsilon^2} H(t, x, \varepsilon B) \right) M_j(t, x, \varepsilon, \varepsilon B) \right]$$

where H is defined by (3) and

$$M_j = (1 + i) \left[\frac{\partial f}{\partial \bar{z}} \cdot \frac{\partial \varphi_t}{\partial p_j} + \frac{f}{i\epsilon^2} \left(-\frac{\partial s}{\partial \bar{z}} \cdot \frac{\partial \varphi_t}{\partial p_j} + \int_0^t \frac{\partial V}{\partial \bar{z}} \cdot \frac{\partial \varphi_s}{\partial p_j} ds \right) \right].$$

In the preceding expression, s, f and their derivatives are evaluated at $\gamma_t^x(t) + \sqrt{i\epsilon}B_t$; the derivatives of V at $\gamma_t^x(s) + \sqrt{i\epsilon}B_s$; and the derivatives of φ at $(x, \dot{\gamma}_t^x(0))$. Moreover, the notation $(\partial f/\partial \bar{z}) \cdot r$ stands for $\sum_{i=1}^d (\partial f/\partial \bar{z}_i) r_i$.

Thus, the almost-analyticity of f, s, V enables us to conclude that

$$\frac{\partial G}{\partial p} \left(\frac{\epsilon^2}{2} A_x \dot{\gamma}_t^x(0) + i \frac{\partial \dot{\gamma}_t^x(0)}{\partial t} \right) = E \left[\exp^{-(1/\epsilon^2) H Z} \left(\frac{\epsilon^2}{2} A_x \dot{\gamma}_t^x(0) + i \frac{\partial \dot{\gamma}_t^x(0)}{\partial t} \right) \right]$$

with Z satisfying (6) and (7).

The same kind of arguments holds for the terms involving $\partial^2 G/\partial q \partial p$, and $\partial^2 G/\partial p^2$. They also have the form $E[\exp(-(1/\epsilon^2) H) Z]$, with Z more complicated than previously, but involving only $\bar{\partial}$ -derivatives of f, s, V . This completes the proof of Lemma 2.5. ■

It remains now to compute $i(\partial G/\partial t) + (\epsilon^2/2) A_q G - (V/\epsilon^2) G$. It is done in

LEMMA 2.6.

$$i \frac{\partial G}{\partial t} + \frac{\epsilon^2}{2} A_q G - \frac{V}{\epsilon^2} G = E \left[Z \exp \left(-\frac{H}{\epsilon^2} \right) \right]$$

where Z satisfies (6) and (7).

Proof of Lemma 2.6. To prove Lemma 2.6, we introduce the process $(X_s(q, p, z, y))_{s \leq t}$, defined by

$$\begin{cases} X_s^1 = \varphi_s(q, p) \\ X_s^2 = \dot{\varphi}_s(q, p) \\ X_s^3 = z + \varphi_s(q, p) - q + \sqrt{i\epsilon}B_s \\ X_s^4 = y - \frac{i}{\epsilon^2} \int_0^s V(X_u^3) du - \frac{1}{\sqrt{i\epsilon}} \int_0^s X_u^2 \delta B_u - \frac{1}{2i\epsilon^2} \int_0^s |X_u^2|^2 du \end{cases}$$

(X_s) is an homogeneous diffusion process with value in $\mathbb{R}^d \times \mathbb{R}^d \times \mathbb{C}^d \times \mathbb{C}$, and with initial condition (q, p, z, y) .

For all suitable function $r: \mathbb{R}^d \times \mathbb{R}^d \times \mathbb{C}^d \times \mathbb{C} \rightarrow \mathbb{R}$, define

$$\Pi_s r(q, p, z, y) = E[r(X_s(q, p, z, y))].$$

For $r(q, p, z, y) = f(z) \exp(+ (i/\varepsilon^2) s(z)) \exp(y)$, we get

$$\Pi_t r(q, p, z, y) \doteq u_t(q, p, z) e^y \quad (13)$$

$$G(t, q, p) \exp(y) = \Pi_t r(q, p, q, y) \quad (14)$$

so that

$$G(t, q, p) = u_t(q, p, q). \quad (15)$$

Itô formula (applied in \mathbb{R}^{4d+2}) gives us the Meyer decomposition of the process $(\Pi_{t-s} r(X_s), s \leq t)$. But, from the Markov property, $(\Pi_{t-s} r(X_s), s \leq t)$ is a martingale. Writing that its bounded variation part is null for $s=0$, yields

$$\begin{aligned} & -\frac{\partial \Pi_t r}{\partial t} + \frac{\partial \Pi_t r}{\partial q} \cdot p - \nabla V(q) \cdot \frac{\partial \Pi_t r}{\partial p} + \frac{\partial \Pi_t r}{\partial z} \cdot p + \frac{\partial \Pi_t r}{\partial y} \cdot \left(\frac{1}{i\varepsilon^2} V(z) - \frac{1}{2i\varepsilon^2} |p|^2 \right) \\ & + \frac{\partial \Pi_t r}{\partial \bar{z}} \cdot p + \frac{\partial \Pi_t r}{\partial \bar{y}} \cdot \left(-\frac{1}{i\varepsilon^2} \bar{V}(z) + \frac{1}{2i\varepsilon^2} |p|^2 \right) + \frac{i\varepsilon^2}{2} \Delta_z \Pi_t r - \frac{i\varepsilon^2}{2} \Delta_{\bar{z}} \Pi_t r \\ & + \varepsilon^2 \Delta_{z, \bar{z}} \Pi_t r + \frac{|p|^2}{2i\varepsilon^2} \frac{\partial^2 \Pi_t r}{\partial y^2} - \frac{|p|^2}{2i\varepsilon^2} \frac{\partial^2 \Pi_t r}{\partial \bar{y}^2} + \frac{|p|^2}{\varepsilon^2} \frac{\partial^2 \Pi_t r}{\partial y \partial \bar{y}} - \frac{\partial^2 \Pi_t r}{\partial y \partial z} \cdot p \\ & + i \frac{\partial^2 \Pi_t r}{\partial y \partial \bar{z}} \cdot p - i \frac{\partial^2 \Pi_t r}{\partial \bar{y} \partial z} \cdot p - \frac{\partial^2 \Pi_t r}{\partial \bar{y} \partial \bar{z}} \cdot p = 0 \end{aligned} \quad (16)$$

where $\Delta_z = \sum_{i=1}^d \partial^2 / \partial z_i^2$, $\Delta_{\bar{z}} = \sum_{i=1}^d \partial^2 / \partial \bar{z}_i^2$, $\Delta_{z, \bar{z}} = \sum_{i=1}^d \partial^2 / \partial z_i \partial \bar{z}_i$, $\partial^2 / \partial y \partial z = (\partial^2 / \partial y \partial z_i)_i$, and so on...

Equation (13) implies that $\partial \Pi_t r / \partial \bar{y} = 0$, and $\partial \Pi_t r / \partial y = \Pi_t r$. (16) reads then

$$\begin{aligned} & -\frac{\partial u_t}{\partial t} + \frac{\partial u_t}{\partial q} \cdot p - \nabla V(q) \cdot \frac{\partial u_t}{\partial p} + \frac{1}{i\varepsilon^2} V(z) u_t \\ & + (1+i) \frac{\partial u_t}{\partial \bar{z}} \cdot p + \frac{i\varepsilon^2}{2} \Delta_z u_t - \frac{i\varepsilon^2}{2} \Delta_{\bar{z}} u_t + \varepsilon^2 \Delta_{z, \bar{z}} u_t = 0. \end{aligned} \quad (17)$$

Using (15), it follows that

$$\begin{aligned} & i \frac{\partial G}{\partial t} + \frac{\varepsilon^2}{2} \Delta_q G - \frac{V}{\varepsilon^2} G \\ & = i \frac{\partial u_t}{\partial q} \cdot p - i \nabla V(q) \cdot \frac{\partial u_t}{\partial p} + \frac{\varepsilon^2}{2} \Delta_q u_t + \varepsilon^2 \Delta_{q, z} u_t + \varepsilon^2 \Delta_{q, \bar{z}} u_t \\ & + (-1+i) \frac{\partial u_t}{\partial \bar{z}} \cdot p + \varepsilon^2 \Delta_{\bar{z}} u_t + (1+i) \varepsilon^2 \Delta_{z, \bar{z}} u_t. \end{aligned} \quad (18)$$

But $u_t(q, p, z) = E[F(z + \varphi(q, p) - q + \sqrt{i\varepsilon}B)$

$$\exp\left(-\frac{1}{\sqrt{i\varepsilon}}\int_0^t \dot{\varphi}_s(q, p) \delta B_s - \frac{1}{2i\varepsilon^2}\int_0^t |\dot{\varphi}_s(q, p)|^2 ds\right)].$$

Apply Lemma 2.4 with $n=4d$, $\theta = (q, p, z) \in \mathbb{R}^d \times \mathbb{R}^d \times \mathbb{C}^d$, and $g(\theta) = z + \varphi(q, p) - q$. Since $\partial g_0^r/\partial p_j = \partial g_0^i/\partial p_j = 0$, $\partial g_0^r/\partial q_j = \partial g_0^i/\partial q_j = 0$, the terms in (18) involving $\partial u_t/\partial p$, $\partial u_t/\partial q$, $\Delta_q u_t$, $\Delta_{q,z} u_t$, $\Delta_{q,\bar{z}} u_t$, have the form $E[\exp^{-1/\varepsilon^2 H} Z]$ with Z satisfying properties (6) and (7) of Proposition 2.2. From $\partial g_0^r/\partial z_j^r = \partial g_0^i/\partial z_j^i = e_j$, and $\partial g_0^r/\partial z_j^i = \partial g_0^i/\partial z_j^r = 0$, we obtain

$$\frac{\partial u_t}{\partial \bar{z}_j} = E\left[\bar{D}F \cdot e_j \exp\left(-\frac{1}{\sqrt{i\varepsilon}}\int_0^t \dot{\varphi}_s \delta B_s - \frac{1}{2i\varepsilon^2}\int_0^t |\dot{\varphi}_s|^2 ds\right)\right].$$

This ends the proof of Lemma 2.6. ■

Proof of Proposition 2.2.3. When the functions f, s, V are analytic on a strip around the real axis, their almost-analytic continuations can be chosen analytic around the real axis. In this case, assertion 3 is satisfied, since Z_j is a function of the $\bar{\partial}$ -derivatives of f, V, s .

This ends the proof of Proposition 2.2. ■

3. SEMI-CLASSICAL EXPANSION OF THE PROBABILISTIC ANSATZ

The aim of this section is to obtain the semi-classical expansion of Ψ . Since Ψ has the form $E[Z \exp(-H/\varepsilon^2)]$, this will be done by the stationary phase method in the Wiener space. For this reason, section 3.1 is devoted to the study of the critical points of the phase function.

3.1. Critical Points of Phase Function

We denote by \mathcal{H}_t the space of continuous paths from $[0, t]$ to \mathbb{R}^d , starting from 0, absolutely continuous with respect to Lebesgue measure on $[0, t]$, and whose derivative is square integrable. \mathcal{H}_t is a Hilbert space, with respect to inner product $\langle h, k \rangle_{\mathcal{H}_t} = \int_0^t \dot{h}_s \cdot \dot{k}_s ds$.

Let us then consider the phase function

$$F_t^{x,r}: \mathcal{H}_t \rightarrow \mathbb{C}$$

$$\begin{aligned} h \mapsto & -is(\gamma_t^x(t) + \sqrt{i}h_t) + i \int_0^t V(\gamma_t^x(s) + \sqrt{i}h_s) ds \\ & + \frac{1}{\sqrt{i}} \int_0^t \dot{\gamma}_t^x(s) \dot{h}_s ds - \frac{i}{2} \int_0^t |\dot{\gamma}_t^x(s)|^2 ds + \frac{1}{2} \int_0^t |\dot{h}_s|^2 ds \quad (19) \end{aligned}$$

The superscript r in $F_t^{x,r}$ recalls the dependence of s and V on r . Therefore, $iF_t^{x,r}$ is just the classical action defined by

$$S_t^x: \mathcal{H}_t \rightarrow \mathbb{R} \tag{20}$$

$$h \mapsto s(x + h_t) - \int_0^t V(x + h_s) ds + \frac{1}{2} \int_0^t |\dot{h}_s|^2 ds$$

taken on the complex path $\gamma_t^x + \sqrt{i}h$. When S_t^x is considered as an operator acting on real paths, it is a well-known fact that its critical points are the classical mechanics trajectories, and that before the caustics, S_t^x has a unique critical point, which is a non degenerate minimum of S_t^x . The question is now to prove that this remains true, when the paths are allowed to visit a neighborhood of the real axis in the complex domain. This is the object of

PROPOSITION 3.7. *Let K be the compact support of f in \mathbb{R}^d . Let us fix $t < T_K$. Then, $\exists r > 0$ such that*

1. $t < T^r \leq T_K$;
2. $\forall x \in K_t^r, h \equiv 0$ is the unique critical point of the phase function $F_t^{x,r}$, and this critical point is non degenerate.
3. $\forall x \in K_t^r, h \equiv 0$ is the unique minimum of the real part of $F_t^{x,r}$, and this minimum is non degenerate.

Proof of Proposition 3.7. The first part of Proposition 3.7 is trivial. Actually, it is sufficient to note that, when $r \rightarrow 0$, K^r decreases to K , and thus T^r increases to T_K .

Let us prove the second assertion of the proposition. Let h and k be elements of \mathcal{H}_t . Denoting by l the complex path $\gamma_t^x + \sqrt{i}h$, we have

$$DF_t^{x,r}(h) \cdot k = -i\sqrt{i} \partial s(l_t) \cdot k_t - i\sqrt{i} \bar{\partial} s(l_t) \cdot k_t$$

$$+ i\sqrt{i} \int_0^t \partial V(l_s) \cdot k_s ds + i\sqrt{i} \int_0^t \bar{\partial} V(l_s) \cdot k_s ds$$

$$+ \frac{1}{\sqrt{i}} \int_0^t \dot{\gamma}_t^x(s) \dot{k}_s ds + \int_0^t \dot{h}_s \dot{k}_s ds$$

$$= -i\sqrt{i} (\partial - i\bar{\partial}) s(l_t) \cdot k_t + \frac{1}{\sqrt{i}} \dot{\gamma}_t^x(t) k_t + \dot{h}_t k_t$$

$$+ i\sqrt{i} \int_0^t (\partial - i\bar{\partial}) V(l_s) \cdot k_s ds - \frac{1}{\sqrt{i}} \int_0^t \ddot{\gamma}_t^x(s) k_s ds - \int_0^t \ddot{h}_s k_s ds$$

$$= -i\sqrt{i} [\dot{l}_t + (\partial - i\bar{\partial}) s(l_t)] \cdot k_t$$

$$+ i\sqrt{i} \int_0^t [\ddot{l}_s + (\partial - i\bar{\partial}) V(l_s)] k_s ds.$$

Thus, h is a critical point of the phase function $F_t^{x,r}$ if and only if $l = \gamma_t^x + \sqrt{i}h$ is solution to

$$\ddot{l}_s + (\partial - i\bar{\partial}) V(l_s) = 0, \quad \forall s \leq t \quad (21)$$

$$l_0 = x \quad (22)$$

$$\dot{l}_t + (\partial - i\bar{\partial}) s(l_t) = 0. \quad (23)$$

From the almost analyticity of V and s , it follows that $\forall z \in \mathbb{R}^d$, $\bar{\partial}V(z) = \bar{\partial}s(z) = 0$, and that $\partial V(z) = \nabla V(z)$, $\partial s(z) = \nabla s(z)$. It is then equivalent to say that $h \equiv 0$ is a critical point, and that γ_t^x satisfies (\mathcal{C}_t^x) .

Let us look at the degeneracy of 0 as a critical point. A straightforward computation leads to

$$\begin{aligned} D^2 F_t^{x,r}(0)(h, h) &= s''(\gamma_t^x(t))(h_t, h_t) - \int_0^t V''(\gamma_t^x(s))(h_s, h_s) ds + \int_0^t |\dot{h}_s|^2 ds \\ &= D^2 S_t^x(\gamma_t^x - x)(h, h) \end{aligned} \quad (24)$$

where the operator S_t^x is the classical action, defined by (20).

But it is a well-known fact that before the caustics (i.e. $t < T_K$), the classical trajectories are non degenerate minima of the action, so that 0 is a non degenerate critical point of $F_t^{x,r}$.

It remains now to prove the uniqueness of 0 as a critical point of $F_t^{x,r}$, at least for small values of r . For this purpose, it is worth to investigate the meaning of the non-degeneracy of 0. First of all, note that

$$D^2 F_t^{x,r}(0)(h, k) = D^2 S_t^x(\gamma_t^x - x)(h, k) = A_t^x(h, k) + \langle h, k \rangle_{\mathcal{H}_t} \quad (25)$$

where the operator A_t^x is defined on \mathcal{H}_t by

$$A_t^x(h, k) = s''(\gamma_t^x(t))(h_t, k_t) - \int_0^t V''(\gamma_t^x(s))(h_s, k_s) ds \quad (26)$$

and satisfies for some constant C (depending on x and t),

$$|A_t^x(h, k)| \leq C \|h\|_t \|k\|_t \quad (27)$$

A_t^x defines thus a continuous quadratic form on the space $\mathcal{C}_0([0, t])$ of continuous paths starting from 0, endowed with uniform convergence. It results then from a result of L. Gross [11], that A_t^x is a trace operator on \mathcal{H}_t , so that there is a basis of \mathcal{H}_t formed by eigenfunctions of A_t^x . The non-degeneracy of γ_t^x means therefore that for all $t < T^r$, and all $x \in K_t^r$, there exists $\alpha_t^x > 0$ such that

$$\forall h \in \mathcal{H}_t, \quad |D^2 F_t^{x,r}(0)(h, h)| \geq \alpha_t^x \|h\|_{\mathcal{H}_t}^2. \quad (28)$$

Moreover, the function $x \mapsto \alpha_t^x$ is lower semi-continuous. Indeed, $\alpha_t^x - 1$ is the lowest eigenvalue of A_t^x , i.e.

$$\alpha_t^x - 1 = \inf\{A_t^x(h, h), h \in \mathcal{H}_t, \|h\|_{\mathcal{H}_t} = 1\} \tag{29}$$

where the extremum is reached, since A_t^x is a trace operator. Thus, $\forall r > 0$, $x \mapsto \alpha_t^x$ reaches its minimum value on the compact set K_t^r . We have then proved the following assertion:

$\forall r > 0$ such that $t < T^r$, there exists $\alpha(r) > 0$, such that

$$\forall x \in K_t^r, \quad \forall h \in \mathcal{H}_t, \quad D^2S_t^x(\gamma_t^x - x)(h, h) \geq \alpha(r)\|h\|_{\mathcal{H}_t}^2. \tag{30}$$

Note that the lower semi-continuity of $x \mapsto \alpha_t^x$ implies that

$$\liminf_{r \rightarrow 0} \alpha(r) \geq \text{Min}_{x \in K_t} \alpha_t^x > 0.$$

We are now going to estimate $D^2F_t^{x,r}(0)$ on a critical point of the phase function $F_t^{x,r}$. Using integration by parts, we can rewrite for all h in \mathcal{H}_t

$$D^2F_t^{x,r}(0)(h, h) = (s''(\gamma_t^x(t)) h_t + \dot{h}_t, h_t) - \int_0^t (\ddot{h}_s + V''(\gamma_t^x(s)) h_s, h_s) ds. \tag{31}$$

When h is a critical point of $F_t^{x,r}$, each of these terms can be evaluated in view of expressions (23) and (21).

Using a Taylor expansion of $(\partial - i\bar{\partial})s(\gamma_t^x(t) + \sqrt{i}h_t)$ around $\gamma_t^x(t)$ to rewrite (23), we obtain

$$\begin{aligned} 0 &= \sqrt{i} (\dot{h}_t + s''(\gamma_t^x(t)) h_t) \\ &+ i \int_0^1 (1-u) \partial^3 s(\gamma_t^x(t) + \sqrt{i}uh_t)(h_t, h_t) du \\ &+ \int_0^1 (1-u) \partial^2 \bar{\partial} s(\gamma_t^x(t) + \sqrt{i}uh_t)(h_t, h_t) du \\ &- i \sqrt{i} \int_0^1 \partial \bar{\partial} s(\gamma_t^x(t) + \sqrt{i}uh_t)(h_t) du - i \bar{\partial} s(\gamma_t^x(t) + \sqrt{i}h_t). \end{aligned}$$

Thus,

$$\begin{aligned} |\dot{h}_t + s''(\gamma_t^x(t)) h_t| \leq &\left\{ C(r) + \sup_{\substack{|y| \leq \sqrt{2}r \\ x \in K^r}} (|\partial^3 s(x + \sqrt{i}y)| \right. \\ &\left. + |\partial^2 \bar{\partial} s(x + \sqrt{i}y)|) \right\} |h_t|^2 \end{aligned}$$

where the constant $C(r)$ comes from the last two terms, and from the almost-analyticity of s . We deduce then that $\forall r > 0$ such that $t < T^r$, there exists $C(r) > 0$ such that $\forall x \in K_t^r, \forall h \in \mathcal{H}_t$ critical point of $F_t^{x,r}$,

$$|\dot{h}_t + s''(\gamma_t^x(t)) h_t| \leq C(r) |h_t|^2. \quad (32)$$

Note that $C(r)$ remains bounded when $r \rightarrow 0$ ($C(r) \xrightarrow{r \rightarrow 0} \sup_{x \in K} |s^{(3)}(x)|$).

We rewrite expression (21) in the same way to obtain that $\forall r > 0$ such that $t < T^r$, there exists $C(r) > 0$ such that $\forall x \in K_t^r, \forall h \in \mathcal{H}_t$ critical point of $F_t^{x,r}, \forall s \leq t$,

$$|\ddot{h}_s + V''(\gamma_t^x(s)) h_s| \leq C(r) |h_s|^2. \quad (33)$$

Again, the constant $C(r)$ remains bounded when $r \rightarrow 0$.

Comparing (32), (33), and (31), it follows that there exists $C_1, C_2 > 0$ such that $\forall r \in]0, 1]$ such that $t < T^r, \forall x \in K_t^r, \forall h \in \mathcal{H}_t$ critical point of $F_t^{x,r}$,

$$\|D^2 F_t^{x,r}(0)(h, h)\| \leq C_1 \|h\|_t^3 \leq C_2 \|h\|_{\mathcal{H}_t}^3. \quad (34)$$

From (30) and (34), it follows that $\exists \alpha > 0, \exists c > 0$ such that $\forall r \in]0, 1]$ such that $t < T^r, \forall x \in K_t^r, \forall h \in \mathcal{H}_t$ critical point of $F_t^{x,r}$ such that $\|h\|_{\mathcal{H}_t} \neq 0$,

$$\alpha \leq C \|h\|_{\mathcal{H}_t}. \quad (35)$$

We need then the following lemma to conclude.

LEMMA 3.8. $\exists \tilde{C} > 0$ such that $\forall r \in]0, 1]$ such that $t < T^r, \forall x \in K_t^r, \forall h \in \mathcal{H}_t$ critical point of $F_t^{x,r}$,

$$\|h\|_{\mathcal{H}_t} \leq \tilde{C}r.$$

Assume that Lemma 3.8 is true, and that $\forall r > 0$, there is a critical point h of $F_t^{x,r}$ such that $\|h\|_{\mathcal{H}_t} \neq 0$. From (35) and Lemma 3.8, it results then that $\alpha \leq C\tilde{C}r$, for all $r \in]0, 1]$.

Therefore, when r is sufficiently small, $h = 0$ is the unique critical point of $F_t^{x,r}$. ■

Proof of Lemma 3.8. Let h be a critical point of $F_t^{x,r}$ such that $\|h\|_{\mathcal{H}_t} \neq 0$. By integration by parts, it follows from (21) and (23) that

$$\begin{aligned} i \|h\|_{\mathcal{H}_t}^2 &= - [\dot{\gamma}_t^x(t) + (\partial - i\bar{\partial}) s(\gamma_t^x(t) + \sqrt{i}h_t)] \sqrt{i}h_t \\ &\quad + \int_0^t [\ddot{\gamma}_t^x(s) + (\partial - i\bar{\partial}) V(\gamma_t^x(s) + \sqrt{i}h_s)] \sqrt{i}h_s ds. \end{aligned} \quad (36)$$

Using (\mathcal{C}_t^x) and a Taylor expansion of $(\partial - i\bar{\partial}) s(\gamma_t^x(t) + \sqrt{i}h_t)$ around $\gamma_t^x(t)$, it follows that

$$\begin{aligned} & |\dot{\gamma}_t^x(t) + (\partial - i\bar{\partial}) s(\gamma_t^x(t) + \sqrt{i}h_t)| \\ & \leq \int_0^1 |(\partial - i\bar{\partial})^2 s(\gamma_t^x(t) + \sqrt{i}uh_t)| |h_t| du \\ & \leq \int_0^1 |(\partial - i\bar{\partial})^2 s(\gamma_t^x(t) + \sqrt{i}uh_t)| \mathbb{1}_{|u| |h_t| \leq \sqrt{2r}} |h_t| du \\ & \leq C_1(r) \int_0^1 \mathbb{1}_{|u| |h_t| \leq \sqrt{2r}} d(u |h_t|) \\ & \leq C_2(r) r \text{ with } C_2(r) \text{ bounded when } r \rightarrow 0. \end{aligned}$$

In the same way, it is easy to prove that $\forall s \leq t$,

$$|\dot{\gamma}_t^x(s) + (\partial - i\bar{\partial}) V(\gamma_t^x(s) + \sqrt{i}h_s)| \leq C_3(r) r, \quad \text{with } C_3(r) \text{ bounded.}$$

Therefore,

$$\|h\|_{\mathcal{H}_t}^2 \leq C_4(r) r \left(|h_t| + \int_0^t |h_s| ds \right) \leq 2C_4(r) r \|h\|_t \leq \tilde{C}(r) \|h\|_{\mathcal{H}_t}$$

so that $\|h\|_{\mathcal{H}_t} \leq \tilde{C}(r) r$.

In order to apply stationary phase method, we have now to look at the global minima of the real part of $F_t^{x,r}$. It is done in exactly the same way as for the critical points of $F_t^{x,r}$, so we omit the proof of the third assertion of Proposition 3.7. ■

3.2. Asymptotic Expansion of Ψ

We are now able to give the asymptotic expansion when $\varepsilon \rightarrow 0$, of Ψ . The result is the following

PROPOSITION 3.9. *Let $t < T_K$, and r be as in Proposition 3.7. For all $x \in \mathbb{R}^d$,*

$$\Psi(t, x) = \exp\left(\frac{i}{\varepsilon^2} S(t, x)\right) \sum_{k=0}^N \beta_k(t, x) \frac{\varepsilon^{2k}}{(2k)!} + O(\varepsilon^{2(N+1)}) \quad (37)$$

where

1. the support of $\beta_k(t, \cdot)$ is included in K_t .
2.
$$\beta_0(t, x) = f(\gamma_t^x(t)) \det(D^2 S_t^x(\gamma_t^x - x))^{-1/2} \quad (38)$$

where S_t^x is defined by (20).

$$3. \quad S(t, x) = S_t^x(\gamma_t^x - x) = s(\gamma_t^x(t)) - \int_0^t V(\gamma_t^x(s)) ds + \frac{1}{2} \int_0^t |\dot{\gamma}_t^x(s)|^2 ds$$

4. the remaining term $O(\varepsilon^{2(N+1)})$ can be understood in any Sobolev norm, or in \mathcal{C}^∞ -norm.

Remark 3.10. It should be noted that although we have given only the expression of the first term β_0 , there is an explicit way of computing all the other terms (see the remark following Lemma 3.12).

Remark 3.11. The usual expression for β_0 is

$$\beta_0(t, x) = \left| \frac{\partial \gamma_t^x(t)}{\partial x} \right|^{1/2} f(\gamma_t^x(t)). \quad (39)$$

To see that (38) and (39) coincide is classical (see for instance [1]).

Proof of Proposition 3.9. It would be sufficient to apply Theorem 7 of [6] to obtain Proposition 3.9. In our context, the proof of this theorem is much easier, so that we give it for the sake of completeness. The main fact is the following lemma, whose proof is given in Appendix 3.

LEMMA 3.12. *Let $t < T_K$, and r be as in Proposition 3.7. Let $L: [0, T] \times \mathbb{R}^d \times \mathcal{W}_t^r \rightarrow \mathbb{R}$ be such that*

1. $\forall x \in \mathbb{R}^d$, the process $L(\cdot, x, \cdot)$ is progressively measurable, and $\forall s \leq t, \forall x \in \mathbb{R}^d, \omega \in \mathcal{W}_s^r \mapsto L(s, x, \omega)$ is \mathcal{C}^∞ .
2. $\forall s \leq t, \forall \omega \in \mathcal{W}_s^r, L(s, \cdot, \omega)$ has compact support in K_s^r .
3. $\forall k \in \mathbb{N}, \sup_{s \leq t} \sup_{x \in \mathbb{R}^d} \sup_{\omega \in \mathcal{W}_s^r} \|D^k L(s, x, \omega)\| < \infty$

where $D^k L$ denotes the k -th derivative of L in ω .

Let us consider for all $s \leq t$, and all $x \in \mathbb{R}^d$,

$$J_\varepsilon(s, x) = E \left[L(s, x, \varepsilon B) \exp \left(-\frac{1}{\varepsilon^2} H(s, x, \varepsilon B) \right) \right].$$

Then,

$$J_\varepsilon(s, x) = \exp \left(\frac{i}{\varepsilon^2} S(s, x) \right) \sum_{p=0}^N \frac{\varepsilon^{2p}}{(2p)!} \beta_p(s, x) + O(\varepsilon^{2(N+1)}) \quad (40)$$

where

- The $O(\varepsilon^{2(N+1)})$ is uniform in $(s, x) \in [0, t] \times \mathbb{R}^d$.
- $\beta_0(s, x) = L(s, x, 0) \det^{-1/2}(D^2 S_s^x(\gamma_s^x - x))$.
- $\beta_p(s, \cdot)$ has compact support in K_s^r .

Moreover, if there exists $r_0 > 0$ such that $\forall s \leq t, \forall \omega, \|\omega\|_s \leq r_0, L(s, x, \omega) \equiv 0$, then $J_\varepsilon(s, x)$ is exponentially small.

Remark 3.13. $\beta_p(s, x)$ can be expressed as

$$\beta_p(s, x) = E[Z_p(s, x) \exp^{-(1/2) A_s^x(B, B)}],$$

where $Z_p(s, x)$ is an element of the $(6p)$ -th Wiener chaos, and A_s^x is defined by (26). It is then possible to compute the expression of β_p in the following way. Let $(f_s^x(i))$ denote an orthonormal basis (in \mathcal{H}_s) of eigenfunctions of A_s^x (eigenvalues $(\alpha_s^x(i))$), and let $(\zeta_s^x(i))$ denote the corresponding basis of the first Wiener chaos. If for all $J = (j_1, \dots, j_m)$,

$$H_J(\zeta_s^x) = \prod_{k=1}^m \frac{1}{\sqrt{j_k!}} H_{j_k}(\zeta_s^x(k))$$

(where H_j is the j -th Hermite polynomial), then $(H_J(\zeta_s^x))_{J=(j_1, \dots, j_m); \sum j_i \leq 6p}$ form a basis of the $6p$ -th Wiener chaos. Therefore, one can write $Z_p(s, x) = \sum_{J, |J| \leq 6p} c_J(s, x) H_J(\zeta_s^x)$. The expression of β_p is then

$$\begin{aligned} \beta_p(s, x) &= \det^{-1/2}(D^2 S_s^x(\gamma_s^x - x)) \sum_{\substack{J=(j_1, \dots, j_m) \\ |J| \leq 6p}} c_J(-1)^m H_J(0) \\ &\quad \times \prod_{k=1}^m \sqrt{\frac{|\alpha_s^x(j_k)|}{1 + \alpha_s^x(j_k)}}. \end{aligned}$$

To get the result of Proposition 3.9 in uniform norm, it is sufficient to apply Lemma 3.12 with $L(s, x, \omega) = f(\gamma_s^x(s) + \sqrt{i}\omega_s)$, which satisfies trivially Assumptions 1–3.

To get the result in \mathcal{C}^1 -norm, let us consider the first derivatives of Ψ . As in Section 2.2, we write that $\Psi(s, x) = G(s, x, \gamma_s^x(0))$. It follows that

$$\frac{\partial \Psi}{\partial x}(s, x) = \frac{\partial G}{\partial q}(s, x, \gamma_s^x(0)) + \frac{\partial G}{\partial p}(s, x, \gamma_s^x(0)) \cdot \frac{\partial \gamma_s^x(0)}{\partial x}.$$

Applying Lemma 2.4, it appears that $\partial \Psi / \partial x(s, x)$ can again be expressed as

$$\sum_{j=-1, 0, 1} \varepsilon^{2j} E \left[L_j(s, x, \varepsilon B) \exp \left(-\frac{H}{\varepsilon^2} \right) \right]$$

where

- For $j = -1, 0, 1, L_j(s, x, \omega)$ satisfies Assumptions 1–3 of Lemma 3.12.
- For $j = -1, 1, \forall k \in \mathbb{N}, \exists C$ such that $\forall x \in K_s^r, \|L_j(s, x, \omega)\| \leq C \|\omega\|_s^k$.

Lemma 3.12 yields then the result of Proposition 3.9 in \mathcal{C}^1 -norm. The same kind of arguments holds for the other derivatives. The assertion concerning the Sobolev norms is then straightforward, since everything happens inside the compact K_r^r .

4. USING THE PROBABILISTIC ANSATZ TO GET SEMI-CLASSICAL ESTIMATES ON THE WAVE FUNCTION

We prove in this section that our probabilistic ansatz is a good approximation of the wave function Φ solution of the Schrödinger equation, in various norms. We begin by the L^2 -norm, for which the hypothesis needed on V is minimal (we just require the Schrödinger operator to be essentially self-adjoint). To get better norms, we have to strengthen our hypothesis on V . We treat the case of H^1 -norm, and uniform norm, but as already said in the introduction, we do not claim here for optimality in our hypothesis on the potential.

4.1. L^2 -Estimates

We will assume in this section that

H4. The operator $A \doteq -(\hbar^2/2)\Delta + V$ defined on C_c^∞ (that is, the set of smooth functions with compact support in \mathbb{R}^d) is essentially self-adjoint. Under this assumption, the Schrödinger equation has a unique solution $\Phi(t, x)$ in $L^2(\mathbb{R}^d, dx)$.

PROPOSITION 4.14. *Let $t < T_K$ and r be as in Proposition 3.7. Under assumptions H1–4, $\forall k \in \mathbb{N}$, $\exists C > 0$ such that*

$$\sup_{s \leq t} \|\Phi(s, \cdot) - \Psi(s, \cdot)\|_{L^2(\mathbb{R}^d, dx)} \leq C\varepsilon^k.$$

Therefore, the semi-classical expansion given in Proposition 3.9 is also valid for Φ in L^2 -norm.

If the functions V, s, f are analytic on a strip around the real axis, the L^2 -error between Ψ and Φ is exponentially small.

Proof of Proposition 4.14. Before proving Proposition 4.14, we are going to demonstrate the following lemma, which will be useful in the sequel.

LEMMA 4.15. *Let $E_s(x)$ and $G_s(x)$ be two functions from $\mathbb{R}^+ \times \mathbb{R}^d$ to \mathbb{C} , such that*

- $\forall s, E_s$ and G_s are in $L^2(\mathbb{R}^d, dx)$.
- $$\begin{cases} ih \frac{\partial E_s}{\partial s}(x) = AE_s(x) + G_s(x) \\ E_0(x) \equiv 0. \end{cases}$$

Let $\tau = \sup\{t, \sup_{s \leq t} \|E_s\|_{L^2(\mathbb{R}^d)} < \infty\}$. Then, for all $t < \tau$,

$$h \sup_{s \leq t} \|E_s\|_{L^2(\mathbb{R}^d)} \leq 2 \int_0^t \|G_u\|_{L^2(\mathbb{R}^d)} du$$

We adopt here the convention that $\sup_{\emptyset} = 0$.

Proof of Lemma 4.15.

$$\begin{aligned} ih \|E_s\|_{L^2(\mathbb{R}^d)}^2 &= ih \|E_0\|_{L^2(\mathbb{R}^d)}^2 + \int_0^s ih \frac{\partial}{\partial u} \|E_u\|_{L^2(\mathbb{R}^d)}^2 du \\ &= \int_0^s \left\langle ih \frac{\partial E_u}{\partial u}, E_u \right\rangle_{L^2(\mathbb{R}^d)} du - \int_0^s \left\langle E_u, ih \frac{\partial E_u}{\partial u} \right\rangle_{L^2(\mathbb{R}^d)} du \end{aligned}$$

where the minus sign comes from the complex conjugation. Thus,

$$\begin{aligned} ih \|E_s\|_{L^2(\mathbb{R}^d)}^2 &= \int_0^s \langle AE_u + G_u, E_u \rangle_{L^2(\mathbb{R}^d)} du - \int_0^s \langle E_u, AE_u + G_u \rangle_{L^2(\mathbb{R}^d)} du \\ &= \int_0^s \langle G_u, E_u \rangle_{L^2(\mathbb{R}^d)} du - \int_0^s \langle E_u, G_u \rangle_{L^2(\mathbb{R}^d)} du \end{aligned}$$

since A is a symmetric operator. Therefore, for all $s \leq t$,

$$h \|E_s\|_{L^2(\mathbb{R}^d)}^2 \leq 2 \int_0^s \|G_u\|_{L^2(\mathbb{R}^d)} \|E_u\|_{L^2(\mathbb{R}^d)} du.$$

Taking the supremum over s , it follows that

$$h(\sup_{s \leq t} \|E_s\|_{L^2(\mathbb{R}^d)})^2 \leq 2(\sup_{s \leq t} \|E_s\|_{L^2(\mathbb{R}^d)}) \int_0^t \|G_u\|_{L^2(\mathbb{R}^d)} du.$$

For $t < \tau$, $h \sup_{s \leq t} \|E_s\|_{L^2(\mathbb{R}^d)} \leq 2 \int_0^t \|G_u\|_{L^2(\mathbb{R}^d)} du$, and the proof of Lemma 4.15 is complete. ■

We return now to the proof of Proposition 4.14. Define for all $s \leq t$ the error function E_s :

$$\begin{aligned} \mathbb{R}^d &\rightarrow \mathbb{C} \\ x &\mapsto \Psi(s, x) - \Phi(s, x). \end{aligned}$$

When $t < T_K \wedge \tau$, Lemma 4.15 and Proposition 2.2 yield

$$\hbar \sup_{s \leq t} \|E_s\|_{L^2(\mathbb{R}^d)} \leq 2t \sup_{s \leq t} \|G_s\|_{L^2(\mathbb{R}^d)}$$

where G_s is the right-hand term in (5), that is

$$G_s(x) = E \left[Z(s, x, \varepsilon, \varepsilon B) \exp \left(-\frac{1}{\varepsilon^2} H(s, x, \varepsilon B) \right) \right]$$

with Z satisfying (6) and (7). We recall that G_s has compact support in K_s^r , so that

$$\begin{aligned} \sup_{s \leq t} \|G_s\|_{L^2(\mathbb{R}^d)} &\leq \text{meas} \left(\bigcup_{s \leq t} K_s^r \right)^{1/2} \sup_{s \leq t} \sup_{x \in K_s^r} |G_s(x)| \\ &\leq \text{meas} \left(\bigcup_{s \leq t} K_s^r \right)^{1/2} \sum_{j=-1, 0, 1} \varepsilon^{2j} \sup_{s \leq t, x \in K_s^r} |E[Z_j \exp^{-H/\varepsilon^2}]| \\ &\leq C(t, \varepsilon, r) \sup_{s \leq t, x \in K_s^r} |E[\exp^{-\Re \varepsilon H/\varepsilon^2}]| \end{aligned}$$

where we have used the estimates (7) on the coefficients Z_j .

Therefore, for all $t < T_K$, $\sup_{s \leq t} \|G_s\|_{L^2(\mathbb{R}^d)} < \infty$. Hence, $\tau \geq T_K$, and $\forall t < T_K$,

$$\hbar \sup_{s \leq t} \|E_s\|_{L^2(\mathbb{R}^d)} \leq 2t \sup_{s \leq t} \|G_s\|_{L^2(\mathbb{R}^d)}.$$

We estimate now $\|G_s\|_{L^2(\mathbb{R}^d)}$ using Lemma 3.12.

$$G_s(x) = \exp \left(\frac{i}{\varepsilon^2} S(s, x) \right) \sum_{j=-1, 0, 1} \sum_{k=0}^{N-j} \alpha_k^j(s, x) \varepsilon^{2(k+j)} + O(\varepsilon^{2(N+1)}).$$

The coefficients α_k^j are defined by

$$\alpha_k^j(s, x) = \frac{1}{(2k)!} E[\theta_j^{(2k)}(s, x, 0)]$$

where $\theta_j^{(2k)}(s, x, \varepsilon)$ is the $(2k)$ -th derivative in ε of

$$\theta_j(s, x, \varepsilon) \equiv Z_j(s, x, \varepsilon B) \exp(-D^2 H(s, x, \varepsilon B)(B \cdot B)).$$

Using the estimates of Z_j given in Proposition 2.2, it follows that $\forall j, \forall k$, $\alpha_k^j(s, x) = 0$.

Furthermore, when f, V, s are analytic in a strip around the real axis, $Z(s, x, \omega) \upharpoonright_{\|\omega\|_s \leq r_0} = 0$; so it follows from Lemma 3.12 that the L^2 -error between Φ and Ψ is exponentially small. ■

4.2. H^1 -Estimates

We consider here the space $H^1(\mathbb{R}^d, dx)$ of functions $f \in L^2(\mathbb{R}^d, dx)$, which are absolutely continuous with respect to Lebesgue measure, and whose derivative is in $L^2(\mathbb{R}^d, dx)$. Instead of H4, we assume here the stronger condition

H5. $V \geq -C_0$ for some constant C_0 .

Under H5, H4 is automatically satisfied (see Theorem 1.1, Chapter 3 in [7]) and the wave function is (as a function of x), in H^1 (see Proposition 1.1, Chapter 3 in [7]).

PROPOSITION 4.16. *Let $t < T_K$ and r be as in Proposition 3.7. Under assumptions H1-3, H5, $\forall k \in \mathbb{N}$, $\exists C > 0$ such that*

$$\|\Phi(t, \cdot) - \Psi(t, \cdot)\|_{H^1(\mathbb{R}^d, dx)} \leq C\varepsilon^k.$$

Therefore, the semi-classical expansion given in Proposition 3.9 is also valid for Φ in H^1 -norm.

Here again, if the functions V, s, f are analytic on a strip around the real axis, the H^1 -error between Ψ and Φ is exponentially small.

Proof of Proposition 4.16. We use the same notations as in the proof of Proposition 4.14.

$$\begin{aligned} \frac{h^2}{2} \|\nabla E_t\|_{L^2}^2 &= \frac{h^2}{2} \int |\nabla E_t(x)|^2 dx \\ &= -\frac{h^2}{2} \langle \Delta E_t, E_t \rangle_{L^2} \\ &= \langle (A - V) E_t, E_t \rangle_{L^2} \\ &\leq \langle A E_t, E_t \rangle_{L^2} + C_0 \|E_t\|_{L^2}^2 \\ &\leq (C_0 + \|A E_t\|_{L^2}) \|E_t\|_{L^2}. \end{aligned}$$

But, $\Psi(t, \cdot)$ and $\Phi(t, \cdot)$ are in the domain of the Schrödinger operator, so that $\|A E_t\|_{L^2} < \infty$. Proposition 4.16 follows then from Proposition 4.14. ■

4.3. Sobolev and \mathcal{C}^∞ -Estimates

The space in consideration is $\mathcal{C}^\infty(\mathbb{R}^d, \mathbb{C})$, i.e. the space of functions $f: \mathbb{R}^d \rightarrow \mathbb{C}$, which are infinitely differentiable. This space is endowed with the uniform norms of f and its derivatives. We will assume that

H6. The derivatives of V of order greater than 2 are bounded, and the wave function Φ is \mathcal{C}^∞ in x with derivatives in $L^2(\mathbb{R}^d, dx)$.

Under H6, H4 is automatically satisfied (see Theorem 1.1, Chapter 3 in [7]).

PROPOSITION 4.17. *Let $t < T_K$ and r be as in Proposition 3.7. Under Assumptions H1-3, H6, $\forall k \in \mathbb{N}$, $\forall l \in \mathbb{N}$, $\exists C > 0$ such that*

$$\sup_{s \leq t} \|\Phi(s, \cdot) - \Psi(s, \cdot)\|_{H^l(\mathbb{R}^d, dx)} \leq C\varepsilon^k.$$

Therefore, the semi-classical expansion given in Proposition 3.9 is valid for Φ in any Sobolev norm, and hence in \mathcal{C}^∞ -norm.

Here again, if the functions V, s, f are analytic on a strip around the real axis, the H^l -error between Ψ and Φ is exponentially small.

Proof of Proposition 4.17. During the proof, we will use the following notations.

- If $M \in \mathbb{N}^d$, $M = (m_1, \dots, m_d)$, $|M| = \sum_{i=1}^d m_i$.
- If $M, L \in \mathbb{N}^d$, $M \oplus L \doteq (m_1 + l_1, \dots, m_d + l_d)$.
- If $M, L \in \mathbb{N}^d$, we say that $L \leq M$ iff $\forall j \in \{1, \dots, d\}$, $l_j \leq m_j$. In this case, we will denote $M \ominus L \doteq (m_1 - l_1, \dots, m_d - l_d)$. Moreover, we will say that $L < M$, iff $L \leq M$, and $\exists j \in \{1, \dots, d\}$ such that $l_j < m_j$.
- If $M \in \mathbb{N}^d$, and $f \in \mathcal{C}^\infty(\mathbb{R}^d, \mathbb{C})$, $D^M f \doteq \partial^{|M|} f / (\partial x_1^{m_1} \dots \partial x_d^{m_d})$.
- If $m, l \in \mathbb{N}$, $l \leq m$, and $f \in \mathcal{C}^\infty(\mathbb{R}^d, \mathbb{C})$,

$$\|f\|_{l,m} \doteq h^{m-l} \sum_{M, |M|=m} \sum_{\substack{L, |L|=l \\ L \leq M}} \left\| \left(\frac{\partial V}{\partial x_1} \right)^{l_1} \dots \left(\frac{\partial V}{\partial x_d} \right)^{l_d} D^{M \ominus L} f \right\|_{L^2}$$

$$\|f\|_m \doteq \sum_{l=0}^m \|f\|_{l,m}$$

$$\| \|f\|_m \doteq \sum_{l=0}^m \|f\|_l.$$

Hence $\| \|f\|_0 = \|f\|_0 = \|f\|_{L^2}$,

$$\|f\|_1 = \sum_{i=1}^d h \left\| \frac{\partial f}{\partial x_i} \right\|_{L^2} + \sum_{i=1}^d \left\| \frac{\partial V}{\partial x_i} f \right\|_{L^2},$$

so that $h \|f\|_{H^1} \leq \| \|f\|_1$ for $h \leq 1$. $\forall m \in \mathbb{N}$, $h^m \|f\|_{H^m} \leq \| \|f\|_m$ for $h \leq 1$.

We are going to prove that all $m \in \mathbb{N}$, $\exists C$ such that $\forall h \leq 1$, $\forall s \leq t$

$$h \sup_{u \leq s} \| \|E_u\| \|_m \leq C \sup_{u \leq s} \| \|G_u\| \|_m. \quad (41)$$

This is done by induction on m . For $m=0$, (41) reduces to

$$h \sup_{u \leq s} \|E_u\|_{L^2} \leq C \sup_{u \leq s} \|G_u\|_{L^2}$$

which has already been proved under assumption H4.

Let us assume that (41) is true for all $n \leq m-1$. Let

$$\tau_m \doteq \sup\{t, \sup_{s \leq t} \|E_s\|_m < \infty\}.$$

We claim that

$$\forall m \geq 1, \exists C \text{ such that } \forall s \leq t, s < \tau_m, \forall h \leq 1,$$

$$h \sup_{u \leq s} \|E_u\|_m \leq C \sup_{u \leq s} \|G_u\|_m + Ch^2 \sup_{u \leq s} \|E_u\|_{m-1}. \quad (42)$$

Thus, the induction hypothesis and (42) allow one to say that $\forall s \leq t$, $s < \tau_m$, $\forall h \leq 1$,

$$h \sup_{u \leq s} \|E_u\|_m \leq C \sup_{u \leq s} \|G_u\|_m.$$

But, exactly in the same way as in the proof of Proposition 4.14, one can see that $\forall t < T_K$, $\sup_{u \leq t} \|G_u\|_m < \infty$. Hence, $\tau_m \geq T_K$, and (41) follows.

Let us prove (42). To this purpose, it is sufficient to show that for all $m \geq 1$, $\forall l \leq m-1$, $\exists C$ such that $\forall s \leq t$, $s < \tau_m$, $\forall h \leq 1$,

$$h \|E_s\|_{l,m} \leq C \sup_{u \leq s} \|G_u\|_m + Ch^2 \sup_{u \leq s} \|E_u\|_{m-1} + Ch \int_0^s \|E_u\|_{l+1,m} du. \quad (43)$$

Indeed, we derive from (43) that $\forall l \leq m-1$,

$$h \|E_s\|_{l,m} \leq C \sup_{u \leq s} \|G_u\|_m + Ch^2 \sup_{u \leq s} \|E_u\|_{m-1} + Ch \int_0^s \|E_u\|_{m,m} du \quad (44)$$

with

$$\|E_u\|_{m,m} = \sum_{M, |M|=m} \left\| \left(\frac{\partial V}{\partial x_1} \right)^{m_1} \cdots \left(\frac{\partial V}{\partial x_d} \right)^{m_d} E_u \right\|_{L^2}.$$

But,

$$\begin{aligned} & ih \frac{\partial}{\partial s} \left(\left[\frac{\partial V}{\partial x_1} \right]^{m_1} \cdots \left[\frac{\partial V}{\partial x_d} \right]^{m_d} E_s \right) \\ &= \left[\frac{\partial V}{\partial x_1} \right]^{m_1} \cdots \left[\frac{\partial V}{\partial x_d} \right]^{m_d} \left(ih \frac{\partial E_s}{\partial s} \right) \end{aligned}$$

$$\begin{aligned}
&= A \left(\left[\frac{\partial V}{\partial x_1} \right]^{m_1} \cdots \left[\frac{\partial V}{\partial x_d} \right]^{m_d} E_s \right) + \left[\left[\frac{\partial V}{\partial x_1} \right]^{m_1} \cdots \left[\frac{\partial V}{\partial x_d} \right]^{m_d} ; -h^2 \Delta \right] E_s \\
&\quad + \left[\frac{\partial V}{\partial x_1} \right]^{m_1} \cdots \left[\frac{\partial V}{\partial x_d} \right]^{m_d} G_s
\end{aligned}$$

where $[B; A]$ denotes the commutator of the operators A and B . Now, for all f, g in $\mathcal{C}^\infty(\mathbb{R}^d, \mathbb{C})$, $[f, -\Delta]g = \Delta fg + 2\nabla f \cdot \nabla g$. Hence, using H6,

$$\left\| \left[\left[\frac{\partial V}{\partial x_1} \right]^{m_1} \cdots \left[\frac{\partial V}{\partial x_d} \right]^{m_d} ; -h^2 \Delta \right] E_s \right\|_{L^2} \leq Ch^2 \|E_s\|_{m-1, m-1} + Ch \|E_s\|_{m-1, m}.$$

Lemma 4.15 then yields that $\forall s \leq t, s \leq \tau_m$,

$$h \|E_s\|_{m, m} \leq C \sup_{u \leq s} \|G_u\|_{m, m} + Ch^2 \sup_{u \leq s} \| \|E_u\| \|_{m-1} + Ch \int_0^s \|E_u\|_{m-1, m} du.$$

Using (43) for $l = m - 1$, it follows then that

$$h \|E_s\|_{m, m} \leq C \sup_{u \leq s} \|G_u\|_m + Ch^2 \sup_{u \leq s} \| \|E_u\| \|_{m-1} + Ch \int_0^s \|E_u\|_{m, m} du.$$

And Gronwall lemma leads to

$$h \sup_{u \leq s} \|E_u\|_{m, m} \leq C \sup_{u \leq s} \|G_u\|_m + Ch^2 \sup_{u \leq s} \| \|E_u\| \|_{m-1}$$

which together with (44), yields (42).

It remains now to show (43). We prove it first for all couples $(0, m)$. We have thus to estimate quantities such as $h^m \|D^M E_s\|_{L^2}$, for $|M| = m$.

$$\begin{aligned}
ih \frac{\partial}{\partial s} (D^M E_s) &= D^M \left(ih \frac{\partial E_s}{\partial s} \right) \\
&= A(D^M E_s) + [D^M; V] E_s + D^M G_s \\
&= A(D^M E_s) + \sum_{J < M} \alpha_M(J) D^{M \ominus J} V D^J E_s + D^M G_s.
\end{aligned}$$

For $|J| \leq |M| - 2$ and $h \leq 1$, $h^m \|D^{M \ominus J} V D^J E_s\|_{L^2} \leq Ch^2 \| \|E_s\| \|_{m-2}$. For $|J| = m - 1$, $h^m \|D^{M \ominus J} V D^J E_s\|_{L^2} \leq h \|E_s\|_{1, m}$. We obtain then from Lemma 4.15, that $\forall s \leq t, s < \tau_m, \forall h \leq 1$,

$$h \|E_s\|_{0, m} \leq C \sup_{u \leq s} \|G_u\|_{0, m} + Ch^2 \sup_{u \leq s} \| \|E_u\| \|_{m-2} + Ch \int_0^s \|E_u\|_{1, m} du$$

that is (43) for $(0, m)$.

Assume now (43) is true for $(l-1, m)$ and let us prove it for (l, m) . We have now to estimate quantities such as $h^{m-l} \|(\partial V/\partial x_1)^{l_1} \dots (\partial V/\partial x_d)^{l_d} D^{M \oplus L} E_s\|_{L^2}$ for $|L| = l$ and $|M| = m$.

$$\begin{aligned}
& ih \frac{\partial}{\partial s} \left(\left[\frac{\partial V}{\partial x_1} \right]^{l_1} \dots \left[\frac{\partial V}{\partial x_d} \right]^{l_d} D^{M \oplus L} E_s \right) \\
&= \left[\frac{\partial V}{\partial x_1} \right]^{l_1} \dots \left[\frac{\partial V}{\partial x_d} \right]^{l_d} ih \frac{\partial}{\partial s} D^{M \oplus L} E_s \\
&= \left[\frac{\partial V}{\partial x_1} \right]^{l_1} \dots \left[\frac{\partial V}{\partial x_d} \right]^{l_d} \left(A(D^{M \oplus L} E_s) \right. \\
&\quad \left. + \sum_{J < M \oplus L} \alpha_{M \oplus L}(J) D^{M \oplus (L \oplus J)} V D^J E_s + D^{M \oplus L} G_s \right) \\
&= A \left(\left[\frac{\partial V}{\partial x_1} \right]^{l_1} \dots \left[\frac{\partial V}{\partial x_d} \right]^{l_d} D^{M \oplus L} E_s \right) + \left[\left[\frac{\partial V}{\partial x_1} \right]^{l_1} \dots \left[\frac{\partial V}{\partial x_d} \right]^{l_d}; -h^2 \Delta \right] D^{M \oplus L} E_s \\
&\quad + \sum_{J < M \oplus L} \alpha_{M \oplus L}(J) \left[\frac{\partial V}{\partial x_1} \right]^{l_1} \dots \left[\frac{\partial V}{\partial x_d} \right]^{l_d} D^{M \oplus (L \oplus J)} V D^J E_s \\
&\quad + \left[\frac{\partial V}{\partial x_1} \right]^{l_1} \dots \left[\frac{\partial V}{\partial x_d} \right]^{l_d} D^{M \oplus L} G_s.
\end{aligned}$$

For $|J| \leq m-l-2$, and $h \leq 1$,

$$h^{m-l} \left\| \left[\frac{\partial V}{\partial x_1} \right]^{l_1} \dots \left[\frac{\partial V}{\partial x_d} \right]^{l_d} D^{M \oplus (L \oplus J)} V D^J E_s \right\|_{L^2} \leq Ch \|E_s\|_{m-2}.$$

For $|J| \leq m-l-1$,

$$h^{m-l} \left\| \left[\frac{\partial V}{\partial x_1} \right]^{l_1} \dots \left[\frac{\partial V}{\partial x_d} \right]^{l_d} D^{M \oplus (L \oplus J)} V D^J E_s \right\|_{L^2} \leq Ch \|E_s\|_{l+1, m}.$$

Moreover,

$$\begin{aligned}
& h^{m-l} \left\| \left[\left[\frac{\partial V}{\partial x_1} \right]^{l_1} \dots \left[\frac{\partial V}{\partial x_d} \right]^{l_d}; -h^2 \Delta \right] D^{M \oplus L} E_s \right\|_{L^2} \\
& \leq Ch^2 \|E_s\|_{l-1, m-1} + Ch \|E_s\|_{l-1, m}.
\end{aligned}$$

By Lemma 4.15, we obtain therefore that for all $s \leq t$, $s \leq \tau_m$, $\forall h \leq 1$,

$$\begin{aligned}
h \|E_s\|_{l, m} &\leq C \sup_{u \leq s} \|G_u\|_{l, m} + Ch^2 \sup_{u \leq s} \|E_u\|_{m-1} \\
&\quad + Ch \int_0^s \|E_u\|_{l+1, m} du + Ch \int_0^s \|E_u\|_{l-1, m} du.
\end{aligned}$$

The induction hypothesis implies then that $\forall s \leq t, s < \tau_m, \forall h \leq 1,$

$$\begin{aligned} h \|E_s\|_{l,m} &\leq C \sup_{u \leq s} \|G_u\|_m + Ch^2 \sup_{u \leq s} \|E_u\|_{m-1} \\ &\quad + Ch \int_0^s \|E_u\|_{l+1,m} du + Ch \int_0^s \|E_u\|_{l,m} du. \end{aligned}$$

And Gronwall lemma leads to (43).

It follows from (41) that

$$h^{m+1} \sup_{s \leq t} \|E_s\|_{H^m} \leq C \sup_{s \leq t} \|G_s\|_m \quad (45)$$

with

$$\|G_s\|_m = \sum_{k=0}^m \sum_{l=0}^k h^{k-l} \sum_{\substack{K, |K|=k \\ L, |L|=l, L \leq K}} \left\| \frac{\partial V^{l_1}}{\partial x_1} \dots \frac{\partial V^{l_d}}{\partial x_d} D^{K \ominus L} G_s \right\|_{L^2}$$

But

$$\|(\partial V^{l_1}/\partial x_1) \dots (\partial V^{l_d}/\partial x_d) D^{K \ominus L} G_s\|_{L^2} \leq C m^{1/2} (K_s^r) \sup_{x \in K_s^r} \|D^{K \ominus L} G_s(x)\|,$$

since G_s has compact support in K_s^r . Therefore,

$$\|G_s\|_m \leq P(h) \sup_{s \leq t} \|G_s\|_{\mathcal{C}^m} \quad (46)$$

where $P(h)$ is a polynomial of degree lower than m . As in the proof of Proposition 4.14, we estimate $\|G_s\|_{\mathcal{C}^m}$ using Lemma 3.12. We obtain that $\forall k \in \mathbb{N}, \exists C$ such that

$$\sup_{s \leq t} \|G_s\|_{\mathcal{C}^m} \leq Ch^k \quad (47)$$

(45), (46) and (47) imply the result of Proposition 4.17. ■

4.4. Localization

It is worth to notice that our probabilistic ansatz Ψ sees only the values of V on a compact set of \mathbb{R}^d , so that it is insensitive to a truncation of V . This truncated potential trivially satisfies the assumptions H6, so that our probabilistic ansatz is an $O(h^\infty)$ approximation in \mathcal{C}^∞ -norm to the wave function associated to this truncated potential. This remark leads us to the definition:

DEFINITION 4.18. We will say that (s, V) is semi-classically localizable in norm $\|\cdot\|$, if for any initial condition f compactly supported, for any T , there is a compact subset K_T of \mathbb{R}^d (depending on (s, V)), and a truncation χ_T (with support in K_T), such that $\|\Phi^V(t, \cdot) - \Phi^{\chi_T V}(t, \cdot)\| = O(h^\infty)$, for $t < T$.

Φ^V denotes here the solution of the Schrödinger equation associated to the potential V .

When (s, V) is semi-classically localizable, our probabilistic ansatz is an $O(h^\infty)$ -approximation of Φ in norm $\|\cdot\|$, whenever

$$\text{For all smooth } f \text{ with compact support, } \exists k, \exists C > 0, \|f\| \leq C \|f\|_{\mathcal{C}^k} \quad (48)$$

In this case, our strategy can be applied to obtain the semi-classical expansion of Φ .

On the other side, to be semi-classically localizable in norm $\|\cdot\|$ is a necessary condition for the semi-classical expansion to be true in norm $\|\cdot\|$ (note that the semi-classical expansion (37) depends only on the values of V on a compact set).

Therefore, for the norms satisfying (48), we have

$$\begin{aligned} (s, V) \text{ semi-classically localizable in norm } \|\cdot\| \\ \Leftrightarrow \text{The semi-classical expansion (37) is valid for } \Phi \text{ in norm } \|\cdot\| \\ \Leftrightarrow \|\Phi - \Psi\| = O(h^\infty) \end{aligned}$$

To determine the class of potentials and initial conditions which are semi-classically localizable in a given norm, is a purely analytical problem. In this section, we have given some answers to this question, but we are aware that these results are certainly not optimal.

APPENDIX 1: PROOF OF PROPOSITION 2.1

Let X_H denote the Hamiltonian vector field associated to V ,

$$\begin{aligned} X_H: \mathbb{R}^d \times \mathbb{R}^d &\rightarrow \mathbb{R}^d \times \mathbb{R}^d \\ (q, p) &\mapsto (p, -\nabla V(q)). \end{aligned}$$

Let $\phi_s(q, p)$ denote the Hamiltonian flow, that is the flow of diffeomorphisms of \mathbb{R}^{2d} associated to X_H . To solve (\mathcal{C}_t^x) is equivalent to look for some initial speed p such that $\phi_t(x, p)$ is in $\mathcal{L}_0 \doteq \{(q, -\nabla s(q)), q \in \mathbb{R}^d\}$. If for all $s \geq 0$, $\mathcal{L}_s \doteq \phi_{-s}(\mathcal{L}_0)$, we have then

$$K_t = \{x \in \mathbb{R}^d, \exists p \text{ such that } (x, p) \in \mathcal{L}_t \text{ and } \pi \circ \phi_t(x, p) \in K\}$$

where π is the first projection in

$$\begin{aligned} \mathbb{R}^{2d}: \mathbb{R}^{2d} &\rightarrow \mathbb{R}^d. \\ (q, p) &\mapsto q. \end{aligned}$$

From the diffeomorphism property of ϕ_t , it is not difficult to see that K_t is a compact subset of \mathbb{R}^d .

Let us consider

$$\begin{aligned} T_K \doteq \sup\{t \geq 0, & \bullet \pi_t = \pi|_{\mathcal{L}_t} \text{ is non singular on } \mathcal{K}_t \doteq \phi_t \pi_0^{-1} K \\ & \bullet \pi_t^{-1}(\pi \mathcal{K}_t) = \mathcal{K}_t\}. \end{aligned}$$

Since \mathcal{L}_0 is projectable, a continuity argument shows that $T_K > 0$. T_K represents the time of *appearance of caustics*. For $t < T_K$, there exists an open neighborhood \mathcal{O}_t of \mathcal{K}_t such that

- π_t is a diffeomorphism from \mathcal{O}_t onto $O_t = \pi(\mathcal{O}_t)$;
- $\pi_t^{-1}(O_t) = \mathcal{O}_t$.

It follows from the definition of T_K , that for $t < T_K$ and $x \in O_t$, there is a unique solution $(\gamma_t^x(s), s \leq t)$ of (\mathcal{C}_t^x) , and that $\gamma_t^x(t) \in K$, whenever $x \in K_t$.

Let us now look at the regularity of γ_t^x in (t, x) . The identity

$$\pi \circ \phi_{-t}(\gamma_t^x(t), -\nabla s(\gamma_t^x(t))) = x$$

holds by construction, so that $\gamma_t^x(t)$ is implicitly defined by $F(t, x, \gamma_t^x(t)) = 0$, where

$$\begin{aligned} F(t, x, y) &= \pi \circ \phi_{-t}(y, -\nabla s(y)) - x \\ &= \pi_t \circ \phi_{-t}(y, -\nabla s(y)) - x. \end{aligned}$$

Now $(\partial F / \partial y)(t, x, y) = T_{\phi_{-t}(y, -\nabla s(y))} \pi_t \circ T_{(y, -\nabla s(y))} \phi_t$ is invertible for all $t < T_K$ and all $y \in O_t$. Therefore, $\gamma_t^x(t)$ has the same regularity in (t, x) as $F(t, x, y)$. It follows that $\gamma_t^x(s) = \pi \circ \phi_{s-t}(\gamma_t^x(t), -\nabla s(\gamma_t^x(t)))$ is \mathcal{C}^∞ in x , and at least \mathcal{C}^1 in t . ■

APPENDIX 2: PROOF OF LEMMA 2.4

$M_s^r(\theta) \doteq \int_0^s \dot{g}_u^r(\theta) \delta B_u$ is a Gaussian process with 0 mean and joint quadratic variation

$$A^r(\theta, \theta', s) = \int_0^s (\dot{g}_u^r(\theta), \dot{g}_u^r(\theta')) du.$$

It follows from the regularity of g that there exists a modification of $(M'_s(\theta))$ which is \mathcal{C}^∞ in $\theta \in \Theta$, and that $\forall \alpha \in \mathbb{N}^n$,

$$D_\theta^\alpha M'_s(\theta) = \int_0^s D_\theta^\alpha \dot{g}'_u \delta B_u$$

(see for instance Theorem 3.1.2, or exercise 3.1.6 of [16]). The same holds for $M'_s(\theta) \doteq \int_0^s \dot{g}'_u \delta B_u$. Therefore,

$$Z_t(\theta) \doteq F(g(\theta) + \sqrt{i\varepsilon}B) \exp\left(-\frac{1}{\sqrt{i\varepsilon}} \int_0^t \dot{g}'_s(\theta) \delta B_s - \frac{1}{2i\varepsilon^2} \int_0^t |\dot{g}'_s(\theta)|_c^2 ds\right)$$

is differentiable in θ , and $\forall j \in \mathbb{N}^m$,

$$\frac{\partial Z}{\partial \theta_j}(\theta) = L_{\theta_j}(F)(\theta, g(\theta) + \sqrt{i\varepsilon}B) \exp\left(-\frac{1}{\sqrt{i\varepsilon}} \int_0^t \dot{g}'_s(\theta) \delta B_s - \frac{1}{2i\varepsilon^2} \int_0^t |\dot{g}'_s(\theta)|_c^2 ds\right)$$

where $\forall \omega \in \mathcal{W}_t(\mathbb{C})$,

$$L_{\theta_j}(F)(\theta, \omega) = D_r F(\omega) \frac{\partial g^r}{\partial \theta_j}(\theta) + D_t F(\omega) \frac{\partial g^i}{\partial \theta_j}(\theta) - \frac{1}{i\varepsilon^2} F(\omega) \int_0^t \frac{\partial \dot{g}'_s}{\partial \theta_j}(\theta) \delta \omega_s.$$

Remark. $\int_0^t (\partial \dot{g}'_s / \partial \theta_j)(\theta) \delta \omega_s$ is defined by integration by parts, since $\partial \dot{g}'_s / \partial \theta_j$ is continuously differentiable.

To invert expectation and differentiation, it is sufficient to prove $\forall \alpha \in \mathbb{N}^n$, $|\alpha| = 2$,

$$\sup_{\theta \in \Theta} E[|D_\theta^\alpha Z_t(\theta)|] < \infty. \tag{49}$$

But, it follows from a computation of the second derivatives and from the hypothesis on F , that $\exists C > 0$ such that $\forall \alpha \in \mathbb{N}^n$, $|\alpha| = 2$,

$$\begin{aligned} E[|D_\theta^\alpha Z_t(\theta)|] &\leq C \left(1 + \sum_{j=1}^n \left\| \exp\left(-\Re e\left(\frac{M_t(\theta)}{\sqrt{i\varepsilon}}\right)\right) \int_0^t \frac{\partial \dot{g}'_s}{\partial \theta_j} \delta B_s \right\|_{L_q} \right. \\ &\quad + \sum_{j,k=1}^n \left\| \exp\left(-\Re e\left(\frac{M_t(\theta)}{\sqrt{i\varepsilon}}\right)\right) \int_0^t \frac{\partial \dot{g}'_s}{\partial \theta_j} \delta B_s \int_0^t \frac{\partial \dot{g}'_s}{\partial \theta_k} \delta B_s \right\|_{L_q} \\ &\quad \left. + \sum_{j,k=1}^n \left\| \exp\left(-\Re e\left(\frac{M_t(\theta)}{\sqrt{i\varepsilon}}\right)\right) \int_0^t \frac{\partial^2 \dot{g}'_s}{\partial \theta_j \partial \theta_k} \delta B_s \right\|_{L_q} \right) \end{aligned}$$

with $1/r + 1/q = 1$. This implies easily (49).

Therefore, G is differentiable in Θ , and $\forall \theta \in \Theta, \forall j \in \{1, \dots, n\}$,

$$\frac{\partial G}{\partial \theta_j} = I_j + J_j \exp\left(-\frac{1}{2i\epsilon^2} \int_0^t |\dot{g}_s|_c^2 ds\right),$$

with

$$I_j = E\left[\left(D_r F \cdot \frac{\partial g^r}{\partial \theta_j} + D_i F \cdot \frac{\partial g^i}{\partial \theta_j}\right) \exp\left(-\frac{1}{\sqrt{i\epsilon}} \int_0^t \dot{g}_s \delta B_s - \frac{1}{2i\epsilon^2} \int_0^t |\dot{g}_s|_c^2 ds\right)\right]$$

$$J_j = E\left[F \cdot \left(-\frac{1}{\sqrt{i\epsilon}} \int_0^t \frac{\partial \dot{g}_s}{\partial \theta_j} \delta B_s - \frac{1}{i\epsilon^2} \int_0^t \frac{\partial \dot{g}_s}{\partial \theta_j} \dot{g}_s ds\right) \exp\left(-\frac{1}{\sqrt{i\epsilon}} \int_0^t \dot{g}_s \delta B_s\right)\right]$$

Consider $l: \mathcal{W}_t \rightarrow \mathbb{C}$, and $K: \mathcal{W}_t \rightarrow \mathcal{W}_t^{*,c}$

$$\omega \mapsto \int_0^t \frac{\partial \dot{g}_s}{\partial \theta_j} \delta \omega_s \quad \omega \mapsto \exp\left(-\frac{1}{\sqrt{i\epsilon}} \int_0^t \dot{g}_s \delta \omega_s\right) l$$

where $\mathcal{W}_t^{*,c}$ is the dual space of \mathcal{W}_t^c . Then, $K = K^r + iK^i$, with $K^r, K^i \in \mathbb{D}_\infty^H$ (see [25] p. 51 for the definition of this space). If δ denotes the dual operator of D defined in corollary of Proposition 1.9 in [25] ($\delta: \mathbb{D}_\infty^H \rightarrow \mathbb{D}_\infty$), then

$$\delta K(\omega) = \exp\left(-\frac{1}{\sqrt{i\epsilon}} \int_0^t \dot{g}_s \delta \omega_s\right) \left[-\int_0^t \frac{\partial \dot{g}}{\partial \theta_j} \delta \omega_s - \frac{1}{\sqrt{i\epsilon}} \int_0^t \frac{\partial \dot{g}_s}{\partial \theta_j} \dot{g}_s ds\right].$$

Thus, a Malliavin integration by parts leads to

$$J_j = -\frac{1}{\sqrt{2i}} E[\langle (D_r + D_i) F(g(\theta) + \sqrt{i\epsilon}B), K(B) \rangle]$$

$$= \frac{-1+i}{\sqrt{2}} E\left[(D_r + D_i) F \cdot \left(\frac{\partial g}{\partial \theta_j} - \frac{\partial g_0}{\partial \theta_j}\right) \exp\left(-\frac{1}{\sqrt{i\epsilon}} \int_0^t \dot{g}_s \delta B_s\right)\right].$$

This proves the identity of the lemma. Moreover, since $\partial G/\partial \theta_j$ has the same form as G , the lemma follows by induction on k .

APPENDIX 3: PROOF OF LEMMA 3.12

We recall that for all s , \mathcal{W}_s is the space $\mathcal{C}([0, s], \mathbb{R}^d)$ endowed with the uniform norm $\|\cdot\|_s$ (associated distance d_s).

Let us write

$$J_\epsilon(s, x) = J_{1,\epsilon}(s, x) + J_{2,\epsilon}(s, x)$$

with

$$J_{1,\varepsilon}(s, x) \equiv E[L(s, x, \varepsilon B) \exp((-1/\varepsilon^2) H(s, x, \varepsilon B)) \mathbb{1}_{\|\varepsilon B\|_s < \rho}].$$

$$J_{2,\varepsilon}(s, x) \equiv E[L(s, x, \varepsilon B) \exp((-1/\varepsilon^2) H(s, x, \varepsilon B)) \mathbb{1}_{\|\varepsilon B\|_s \geq \rho}].$$

We are going to show that $J_{2,\varepsilon}$ is exponentially small, and that $J_{1,\varepsilon}$ gives the asymptotic expansion (40).

Treatment of $J_{1,\varepsilon}$. $H(s, x, 0) = -iS(s, x)$, $DH(s, x, 0) = DF_s^{x,r}(0) = 0$, since 0 is critical point of $F_s^{x,r}$. A Taylor expansion of $\varepsilon \mapsto H(s, x, \varepsilon B)$ yields then

$$J_{1,\varepsilon}(s, x) = e^{(i/\varepsilon^2) S(s, x)} E[L(s, x, \varepsilon B) e^{-A(s, x, \varepsilon)} \mathbb{1}_{\|\varepsilon B\|_s < \rho}] \tag{50}$$

where $A(s, x, \varepsilon) = \int_0^1 (1-v) D^2H(s, x, \varepsilon v B)(B, B) dv$, is \mathcal{C}^∞ in ε .

Let us write now the Taylor expansion of $\theta(s, x, \varepsilon) = L(s, x, \varepsilon B) e^{-A(s, x, \varepsilon)}$ around $\varepsilon = 0$. We obtain

$$\theta(s, x, \varepsilon) = \sum_{k=0}^N \frac{\varepsilon^k}{k!} \tilde{Z}_k(s, x) + \varepsilon^{N+1} R(s, x, \varepsilon) \tag{51}$$

with

$$\tilde{Z}_k(s, x) = Z_k(s, x) e^{-A(s, x, 0)} = Z_k(s, x) e^{-(1/2) A_s^x(B, B)}$$

where $Z_k(s, x)$ is a sum of terms such as $C(s, x)(B, \dots, B)$, with $C(s, x)$ any deterministic multilinear functional of order lower than $6k$ on the Wiener space \mathcal{W}_s . Hence, $Z_k(s, x)$ is an element of the $(6k)$ -th Wiener chaos. The coefficients of $C(s, x)$ involve the derivatives of $L(s, x, \cdot)$ at 0, and the derivatives of order greater than 2 of $H(s, x, \cdot)$ at 0. Using Assumption 2, it is easily checked that for all $s \leq t$, $C(s, \cdot)$ has compact support in K_s^r , so that the same is true for $\tilde{Z}_k(s, \cdot)$, and for $R(s, \cdot, \varepsilon)$ by (51). Moreover, assumption 3 yields that $\forall p \geq 0$,

$$\sup_{s \leq t} \sup_{x \in K_s^r} E[|Z_k(s, x)|^p] < \infty \tag{52}$$

It follows then from (50) and (51) that

$$e^{-(i/\varepsilon^2) S(s, x)} J_{1,\varepsilon}(s, x) = \sum_{k=0}^N \frac{\varepsilon^k}{k!} E(\tilde{Z}_k(s, x)) + \sum_{k=0}^N \frac{\varepsilon^k}{k!} E(\tilde{Z}_k(s, x) \mathbb{1}_{\|\varepsilon B\|_s \geq \rho}) + \varepsilon^{N+1} E(R(s, x, \varepsilon) \mathbb{1}_{\|\varepsilon B\|_s < \rho}). \tag{53}$$

The first sum gives the semi-classical expansion (40), if we put $\beta_k(s, x) = E(\tilde{Z}_k(s, x))$. We have indeed already prove that $\beta_k(s, \cdot)$ has compact

support in K_s^r . Moreover, by symmetry of Brownian motion, $\beta_k(s, x) = 0$ for odd k . Let us then compute β_0 .

$$\beta_0(s, x) = E(Z_0(s, x) e^{(-1/2) A_s^x(B, B)}) = L(s, x, 0) E(e^{(-1/2) A_s^x(B, B)})$$

$A_s^x(B, B)$ is an element of the second Wiener chaos. Let us write its decomposition

$$A_s^x(B, B) = \sum_k \alpha_s^x(k) \zeta_k^2(s, x)$$

where $(\zeta_k(s, x))_{k \geq 1}$ are i.i.d $\mathcal{N}(0, 1)$ random variables, and $(\alpha_s^x(k))_{k \geq 1}$ are the eigenvalues of the trace-class operator A_s^x (in increasing order). Since $t < T^r$, we have already seen that $\forall s \leq t, \forall x \in K_s^r, \forall k \in \mathbb{N}, 1 + \alpha_s^x(k) > 0$. Therefore

$$E(e^{(-1/2) A_s^x(B, B)}) = \prod_{k=1}^{\infty} (1 + \alpha_s^x(k))^{-1/2} = \det^{-1/2}(D^2 S_s^x(\gamma_s^x - x))$$

since $D^2 S_s^x(\gamma_s^x - x) = A_s^x + \text{Id}$. Note that this product is finite by the trace property. For the computation of the other terms, the reader is referred to [6].

We are now going to prove that the second sum in (53) is exponentially small.

$$\begin{aligned} & \sup_{\substack{s \leq t \\ x \in K_s^r}} |E[\tilde{Z}_k(s, x) \mathbb{1}_{\|\varepsilon B\|_s \geq \rho}]| \\ & \leq \sup_{\substack{s \leq t \\ x \in K_s^r}} |E[Z_k(s, x) e^{(-1/2) A_s^x(B, B)} \mathbb{1}_{\|\varepsilon B\|_s \geq \rho}]| \\ & \leq \sup_{\substack{s \leq t \\ x \in K_s^r}} E[|Z_k(s, x)|^{p_1}]^{1/p_1} \sup_{\substack{s \leq t \\ x \in K_s^r}} E[e^{(-p_2/2) A_s^x(B, B)}]^{1/p_2} \\ & \quad \times P[\|\varepsilon B\|_t \geq \rho]^{1/p_3} \end{aligned} \tag{54}$$

with $1/p_1 + 1/p_2 + 1/p_3 = 1, p_i > 1$. The first term in the right-hand side is finite using (52). Furthermore,

$$P[\|\varepsilon B\|_t \geq \rho]^{1/p_3} \leq \exp\left(-\frac{\rho^2}{2p_3 t \varepsilon^2}\right).$$

Thus, our goal is achieved as soon as we have found $p_2 > 1$ such that the second term in the right-hand side of (54) is finite. From the lower semi-continuity of $(s, x) \mapsto \alpha_s^x(1)$, it follows that

$$\text{Min}_{s \leq t} \text{Min}_{x \in K_s^r} \alpha_s^x(1) > -1$$

so that one can found $p_2 > 1$, such that

$$\text{Min}_{s \leq t} \text{Min}_{x \in K_s^r} \alpha_s^x(1) > -\frac{1}{p_2} > -1.$$

It implies that $\forall s \leq t, \forall x \in K_s^r$,

$$E \left[\exp \left(-\frac{p_2}{2} A_s^x(B, B) \right) \right] = \prod_{k=1}^{\infty} \frac{1}{\sqrt{1 + p_2 \alpha_s^x(k)}} < \infty$$

Fatou’s lemma yields that the function $(s, x) \mapsto E[\exp(- (p_2/2) A_s^x(B, B))]$ is lower semi-continuous, and reaches therefore its maximum value on any compact set. Hence,

$$\sup_{\substack{s \leq t \\ x \in K_s^r}} E \left[\exp \left(-\frac{p_2}{2} A_s^x(B, B) \right) \right] < \infty$$

It remains now to treat $E[R(s, x, \varepsilon) \mathbb{1}_{\|eB\|_s < \rho}]$,

$$R(s, x, \varepsilon) = \int_0^1 \frac{(1-v)^N}{N!} \frac{\partial^{N+1}}{\partial \varepsilon} \theta(s, x, \varepsilon v) dv$$

with $(\partial^{N+1}/\partial \varepsilon) \theta(s, x, \varepsilon v) = M(s, x, \varepsilon v B) e^{-A(s, x, \varepsilon v)}$ and $\forall p > 1, \sup_{s \leq t, x \in K_s^r} \sup_{v \in [0, 1]} E[|M(s, x, \varepsilon v B)|^p] < \infty$. Let us choose q such that $1 < q < p_2$, and let p be the conjugate of q .

$$\begin{aligned} \sup_{\substack{s \leq t \\ x \in K_s^r}} |E[R(s, x, \varepsilon) \mathbb{1}_{\|eB\|_s < \rho}]| &\leq \int_0^1 \frac{(1-v)^N}{N!} \sup_{\substack{s \leq t \\ x \in K_s^r}} E[|M(s, x, \varepsilon v B)|^p]^{1/p} \\ &\quad \times \sup_{\substack{s \leq t \\ x \in K_s^r}} E[e^{-q \Re e A(s, x, \varepsilon v)} \mathbb{1}_{\|eB\|_s < \rho}]^{1/q} dv \\ &\leq C \sup_{\substack{s \leq t \\ x \in K_s^r}} \sup_{v \in [0, 1]} E[e^{-q \Re e A(s, x, \varepsilon v)} \mathbb{1}_{\|eB\|_s < \rho}]^{1/q} \end{aligned}$$

But $A(s, x, \varepsilon v) = \frac{1}{2} A_s^x(B, B) + v \int_0^1 (1-u)^2 / 2 D^3 H(s, x, \varepsilon u v B)(\varepsilon B, B, B) du$, so that

$$|\Re e A(s, x, \varepsilon v) - \frac{1}{2} A_s^x(B, B)| \mathbb{1}_{\|eB\|_s < \rho} \leq C \rho \|B\|_s^2$$

where the constant C can be chosen uniform in (s, x, v) , $s \leq t$, $x \in K_s^r$, $v \in [0, 1]$. Therefore,

$$\begin{aligned}
& \sup_{\substack{s \leq t \\ x \in K_s^r}} \sup_{v \in [0, 1]} E[\exp(-q \Re e A(s, x, \varepsilon v)) \mathbb{1}_{\|\varepsilon B\|_s < \rho}] \\
& \leq \sup_{\substack{s \leq t, v \in [0, 1] \\ x \in K_s^r}} E[e^{-(q\rho_2/p_2 - q)(\Re e A(s, x, \varepsilon v) - (1/2) A_s^{\chi}(B, B))}]^{(p_2 - q)/p_2} \\
& \quad \times \sup_{\substack{s \leq t \\ x \in K_s^r}} E[e^{-(p_2/2) A_s^{\chi}(B, B)}]^{q/p_2} \\
& \leq CE[e^{C\rho \|B\|_t^2}] < \infty \quad \text{as soon as} \quad \rho < \frac{1}{2Ct}.
\end{aligned}$$

We have thus proved that $\exists \rho_0 > 0$, such that $\forall \rho \leq \rho_0$

$$J_{1, \varepsilon}(s, x) = \exp\left(\frac{i}{\varepsilon^2} S(s, x)\right) \sum_{k=0}^N \beta_k(s, x) \frac{\varepsilon^k}{k!} + O(\varepsilon^{N+1}) \quad (55)$$

where the $O(\varepsilon^{N+1})$ is uniform in (s, x) .

Treatment of $J_{2, \varepsilon}$. From now on, we fix ρ such as (55) holds. Here are some notations we use in the sequel

- When

$$\begin{aligned}
s \leq t, \quad A_s: \mathcal{W}_s \rightarrow \overline{\mathbb{R}} \\
\omega \mapsto \begin{cases} \frac{1}{2} \|\omega\|_{\mathcal{H}_s}^2 & \text{if } \omega \in \mathcal{H}_s \\ +\infty & \text{otherwise} \end{cases}
\end{aligned}$$

is the rate function for the large deviations of Brownian motion. A_s is lower semi-continuous, and the level sets of A_s are compact.

- When $k > 0$, $C_k^s = \{\omega \in \mathcal{W}_s, A_s(\omega) \leq k\}$,
- When $k > 0$, and $\delta > 0$, $C_k^s(\delta) = \{\omega \in \mathcal{W}_s, d_s(\omega, C_k^s) < \delta\}$.

As being a good rate function, $C_k^s \cap \{\|\omega\|_s \geq \rho\}$ is a compact subset of \mathcal{W}_s . Thus the lower semi-continuous function $\omega \in \mathcal{W}_s \mapsto \Re e H(s, x, \omega) + A_s(\omega)$ reaches its minimum value $m(s, x)$ on $C_k^s \cap \{\|\omega\|_s \geq \rho\}$. Since $s < T^r$, we know by Proposition (3.7) that the unique global minimum of $\Re e H(s, x, \cdot) + A_s(\cdot) = \Re e F_s^{x, r}$ is 0. Therefore for all $s \leq t$, and all $x \in K_s^r$, $m(s, x) > 0$. The function $(s, x) \mapsto m(s, x)$ being lower semi-continuous, $\exists m > 0$ such that $\forall s \leq t$, $\forall x \in K_s^r$, $\forall \omega \in C_s^k \cap \{\|\omega\|_s \geq \rho\}$, $\Re e H(s, x, \omega) + A_s(\omega) \geq m$.

Let us fix \tilde{m} such that $0 < \tilde{m} < m$. By the lower semi-continuity of $H + A_s$, we obtain $\delta_0 > 0$ and $\eta_0 < \rho$ such that $\forall \delta < \delta_0, \forall \eta, \eta_0 < \eta < \rho, \forall s \leq t, \forall x \in K_s^r, \forall \omega \in C_s^k(\delta), \|\omega\|_s \leq \rho - \eta, \Re H(s, x, \omega) + A_s(\omega) \geq \tilde{m}$. For such (δ, η) , let us write

$$\begin{aligned}
 |J_{2,\varepsilon}(s, x)| &\leq E \left[\exp \left(-\frac{\Re H(s, x, \varepsilon B)}{\varepsilon^2} \right) \mathbb{1}_{\|\varepsilon B\|_s \geq \rho} \right] \\
 &\leq E \left[\exp \left(-\frac{\Re H(s, x, \varepsilon B)}{\varepsilon^2} \right) \mathbb{1}_{\|\varepsilon B\|_s > \rho - \eta} \mathbb{1}_{\varepsilon B \in C_s^k(\delta)} \right] \\
 &\quad + E \left[\exp \left(-\frac{\Re H(s, x, \varepsilon B)}{\varepsilon^2} \right) \mathbb{1}_{\|\varepsilon B\|_s \geq \rho} \mathbb{1}_{d_s(\varepsilon B, C_s^k) \geq \delta} \right]. \tag{56}
 \end{aligned}$$

Let us treat the second term in the right-hand side of (56)

$$\begin{aligned}
 \Re H(s, x, \varepsilon B) &= \Im s(\gamma_s^x(s) + \sqrt{i\varepsilon}B_s) - \int_0^s \Im mV(\gamma_s^x(u) + \sqrt{i\varepsilon}B_u) du \\
 &\quad + \frac{\sqrt{2}}{2} \int_0^s \dot{\gamma}_s^x(u) \delta(\varepsilon B_u).
 \end{aligned}$$

Therefore, $\exists A > 0$ such that $\forall s \leq t, \forall x \in K_s^r$,

$$\begin{aligned}
 &E \left[\exp \left(-\frac{\Re H(s, x, \varepsilon B)}{\varepsilon^2} \right) \mathbb{1}_{\|\varepsilon B\|_s \geq \rho} \mathbb{1}_{d_s(\varepsilon B, C_s^k) \geq \delta} \right] \\
 &\leq \exp \left(\frac{A}{\varepsilon^2} \right) E \left[\exp \left(-\frac{\sqrt{2}}{2\varepsilon} \int_0^s \dot{\gamma}_s^x(u) \delta B_u \right) \mathbb{1}_{d_s(\varepsilon B, C_s^k) \geq \delta} \right] \\
 &\leq \exp \left(\frac{A}{\varepsilon^2} \right) E \left[\exp \left(-\frac{\sqrt{2}}{\varepsilon} \int_0^s \dot{\gamma}_s^x(u) \delta B_u \right) \right]^{1/2} P[d_s(\varepsilon B, C_s^k) \geq \delta]^{1/2} \\
 &\leq \exp \left(\frac{A}{\varepsilon^2} \right) \exp \left(\frac{1}{\varepsilon^2} \int_0^s |\dot{\gamma}_s^x(u)|^2 du \right) P[d_t(\varepsilon B, C_t^k) \geq \delta]^{1/2} \\
 &\leq \exp \left(\frac{\tilde{A}}{\varepsilon^2} \right) P[\varepsilon B \notin C_t^k(\delta)]^{1/2}
 \end{aligned}$$

where the constant \tilde{A} does not depend on (s, x) . $C_t^k(\delta)$ is an open set of \mathcal{W}_t , an the large deviations for the Brownian motion yield (for ε sufficiently small),

$$\begin{aligned}
 P[\varepsilon B \notin C_t^k(\delta)] &\leq \exp \left(-\frac{1}{\varepsilon^2} \inf_{\omega \notin C_t^k} A_t(\omega) \right) \\
 &\leq \exp \left(-\frac{k}{\varepsilon^2} \right)
 \end{aligned}$$

for δ sufficiently small. It is then sufficient to take $k > \tilde{A}$ to obtain the exponential decay.

It remains now to treat the first term in the right-hand side of (56). Let us choose \bar{m} , such that $0 < \bar{m} < \tilde{m}$, and let us define

$$H_1: [0, t] \times \mathbb{R}^d \times \mathcal{W}_t \rightarrow \mathbb{R}$$

$$(s, x, \omega) \mapsto \begin{cases} \Re H(s, x, \omega) & \text{if } \omega \in C_s^k(\delta) \text{ and } \|\omega\|_s > \rho - \eta \\ \bar{m} - A_s(\omega) & \text{otherwise.} \end{cases}$$

Since $C_s^k(\delta) \cap \{\omega, \|\omega\|_s > \rho - \eta\}$ is an open set of \mathcal{W}_s , $\omega \in \mathcal{W}_s \mapsto H_1(s, x, \omega)$ is lower semi-continuous $\forall s \leq t, \forall x \in \mathbb{R}^d$. Moreover,

$$E \left[\exp \left(-\frac{\Re H(s, x, \varepsilon B)}{\varepsilon^2} \right) \mathbb{1}_{\varepsilon B \in C_s^k(\delta)} \mathbb{1}_{\|\varepsilon B\|_s > \rho - \eta} \right]$$

$$\leq E \left[\exp \left(-\frac{H_1(s, x, \varepsilon B)}{\varepsilon^2} \right) \right]$$

Using corollary 2.9 in [21] (which can be rendered uniform in (s, x)), we obtain that $\forall s \leq t, \forall s \in K_s^r$, for ε sufficiently small

$$E \left[\exp \left(-\frac{H_1(s, x, \varepsilon B)}{\varepsilon^2} \right) \right] \leq \exp \left(-\frac{\bar{m}}{\varepsilon^2} \right)$$

The proof of Lemma 3.12 is thus complete.

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