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A case study on the reliability of multiphase WKB approximation for the one-dimensional Schrödinger equation

*Laurent Gosse**

Abstract. We present a short overview of high-frequency asymptotics for the 1D Schrödinger equation while emphasizing the computational aspects. We show that presumably different techniques like stationary phase methods, WKB or Wigner analysis give essentially the same macroscopic behaviour. Moment systems and K-branch entropy solutions are introduced in order to derive well-suited numerical methods. Finally, we display some computations supporting these ideas on a classical example.

1. Introduction

We are interested in computing efficiently the high frequency asymptotics of the Cauchy problem for the following linear equation:

$$i\hbar\partial_t\psi + \frac{\hbar^2}{2m}\partial_{xx}\psi = 0, \quad \psi(t=0, \cdot) = \psi_0; \quad x \in \mathbb{R}. \quad (1.1)$$

The unknown ψ is the quantum mechanical wave-function of some particle of mass $m > 0$; \hbar stands of course for the Planck constant. It is customary to work with dimensionless variables and one is led to introduce a *scaled Planck constant* $\varepsilon > 0$; problem (1.1) rewrites

$$i\varepsilon\partial_t\psi + \frac{\varepsilon^2}{2}\partial_{xx}\psi = 0, \quad \psi(t=0, \cdot) = \psi_0; \quad x \in \mathbb{R}. \quad (1.2)$$

In order to study the wave-particle transition (or *classical limit*), one is especially interested in a class of initial data of the WKB (or *monokinetic*) type:

$$\psi(t=0, \cdot) = A_0(x) \exp(i\varphi_0(x)/\varepsilon); \quad x \in \mathbb{R}. \quad (1.3)$$

The slowly-varying quantities $A_0 \geq 0$ and φ_0 appearing in this last expression are called respectively the amplitude and the phase of the wave ψ_0 . Data of the form (1.3) with A_0 compactly supported are usually called *wave packets*. We stress that the equation (1.2) may arise when considering areas of application different from quantum mechanics, see [26].

2. Asymptotics of ψ and rays

In this section, we aim at setting up techniques in order to compute the asymptotics of ψ satisfying (1.2)–(1.3) for $\varepsilon \rightarrow 0$ without solving numerically the equation in order to bypass the meshing constraints explained in [23].

2.1. The stationary phase method

This procedure is extensively exposed in [8]; we have in mind to present it briefly in our rather simple context. A first and elementary observation is that the scaled Schrödinger equation (1.2)–(1.3) admits an explicit solution in terms of a so-called *oscillatory integral*:

$$\psi(t, x) = \int_{\mathbb{R}} \int_{\mathbb{R}} A_0(y) \exp\left(\frac{i}{\varepsilon} \left(\varphi_0(y) + \xi(x - y) - t\xi^2/2\right)\right) .dy.d\xi. \quad (2.4)$$

We call "generalized phase" the function $S(\xi, y) = \varphi_0(y) + \xi(x - y) - t\xi^2/2$ in order to avoid any confusion with the aforementioned WKB phase φ . Then the stationary phase lemma ensures that provided A_0, φ_0 are C^∞ functions,

$$\psi(t, x) = \sum_j \frac{A_0(y_j)}{\sqrt{1 + t\varphi_0''(y_j)}} \exp\left(\pm \frac{i\pi}{4}\right) \exp\left(\frac{i}{\varepsilon} \left(\varphi_0(y_j) + t\varphi_0(y_j)^2/2\right)\right) + O(\varepsilon). \quad (2.5)$$

Loosely speaking, one goes from a continuous superposition of waves in (2.4) to a discrete one (2.5) discarding all the couples of points ξ, y except those around which the generalized phase S is stationary thanks to the numerous cancellations inside the integral. The selected points are therefore critical points of S hence

$$\nabla_{\xi, y} S = 0 \Leftrightarrow \varphi_0'(y) - \xi = 0, \quad x - y - t\xi = 0.$$

So, for any $x \in \mathbb{R}$ and at a given time $t > 0$, one has to find all the possible values $y_j, j = 1, 2, 3, \dots$ satisfying the **ray equations** (also called bicharacteristics)

$$\xi = \varphi_0'(y), \quad x = y + t\varphi_0'(y). \quad (2.6)$$

In the language of conservation laws, one is more used to speak about characteristic curves; in this case, φ_0' is related to the initial velocity, as we shall see later.

A central problem in this approach is that the approximation (2.5) seems to blow up for $1 + t\varphi_0''(y_j) \rightarrow 0$; we shall call this blow-up locus the **caustic curve**.

2.2. Wigner measure analysis

A more modern tool to investigate the classical limit of (1.2)–(1.3) is the Wigner transform, which is defined as an "angularly resolved energy density":

$$W[\psi](t, x, \xi) = \int_{\mathbb{R}} \psi(t, x + \varepsilon z/2) \bar{\psi}(t, x - \varepsilon z/2) \exp(-i\xi z) dz. \quad (2.7)$$

Let us define a sequence of solutions ψ^ε to (1.2)–(1.3) and W^ε its associated family of Wigner transforms; then a well-known compactness lemma, [21], states that

$$\|\psi^\varepsilon\|_{L^2} \leq C \text{ uniformly} \Rightarrow W^\varepsilon \rightharpoonup W \in \mathcal{M}^+, \quad \varepsilon \rightarrow 0,$$

where \mathcal{M}^+ stands for the cone of nonnegative measures in $t, x, \xi \in \mathbb{R}^+ \times \mathbb{R} \times \mathbb{R}$. Moreover, the limit Wigner measure satisfies the following free transport equation,

$$\partial_t W + \xi \partial_x W = 0, \quad W(t=0, x, \xi) = A_0(x)^2 \delta(x - \partial_x \varphi_0(x)), \quad (2.8)$$

($\delta(\cdot)$ the standard Dirac measure) which admits the explicit solution,

$$W(t, x, \xi) = W(t=0, y, \xi),$$

away from caustics, as soon as for any $x \in \mathbb{R}$ and at a given time $t > 0$, y satisfies the ray equations (2.6). Of course, one shouldn't expect a unique solution in the general case; thus several values y_j , $j = 1, 2, 3, \dots$ are to be found. Accordingly, the initial monokinetic density will split into a more complex object of the type (2.5) beyond a certain **breakup time**.

A major interest in this technique lies in the fact that quadratic observables can be easily obtained by taking the moments of W ; for instance, the position density reads:

$$\rho(t, x) = \lim_{\varepsilon \rightarrow 0} |\psi^\varepsilon(t, x)|^2 = \int_{\mathbb{R}} W(t, x, \xi) d\xi. \quad (2.9)$$

2.3. WKB and the evolution of the position density

This technique is based on the assumption that for any value of the scaled Planck constant ε below a certain threshold, the solution of (1.2)–(1.3) is well approximated by an ansatz,

$$\psi(t, x) \simeq A(t, x) \exp(i\varphi(t, x)/\varepsilon), \quad t > 0.$$

Another convenient way to motivate this ansatz is to trace back to (2.5) while introducing a (generally multivalued) mapping $Y : (t, x) \mapsto y_j$, $j = 1, 2, \dots$ such that equations (2.6) hold. Finally, one defines a phase-amplitude pair $\varphi(t, x), A(t, x)$ relying on (2.5) and the quantities $y_j = Y(t, x)$. In modern language, working with an ansatz amounts to guessing the microstructure in the problem (1.2)–(1.3); it says that the fine scale structure of the initial data stands still forever. Indeed, the scaling in (2.7) is adapted to wave functions ψ endowed with oscillations of $O(\varepsilon)$ wave-length.

Thus plugging this ansatz and splitting between real and imaginary parts inside (1.2) leads to:

$$\partial_t \varphi + \frac{1}{2}(\partial_x \varphi)^2 = \frac{\varepsilon^2}{2A} \partial_{xx} A, \quad \partial_t(A^2) + \partial_x(A^2 \partial_x \varphi) = 0. \quad (2.10)$$

The "act of faith" that leads to the classical WKB system is that $\frac{\varepsilon^2}{2A} \partial_{xx} A \rightarrow 0$ when $\varepsilon \rightarrow 0$; this **dispersive limit** is essentially supported beyond breakup time by the fact that the emerging eikonal equation on φ admits the same rays as (2.6). So there is a consistency with the two preceding methods. Let us also recall that for small time, this kind of asymptotics are fully justified, see [16]. A survey is also given by Keller [20]

In the limit, system (2.10) becomes weakly coupled as the eikonal equation decouples and can be solved independently; of course, in order to remain consistent with the two aforementioned procedures, one must give up the idea of solving in the context of *viscosity solutions*, [7]. See however [12] for rather complete results in this (wrong) direction. If one introduces a velocity variable $u = \partial_x \varphi$, then the first equation becomes the classical Burgers' equation

$$\partial_t u + u \partial_x u = 0, \quad u_0 = \partial_x \varphi_0,$$

for which the multivalued (or geometric) solution is to be sought through the rays (2.6), [4, 17]. If one can complete this program, then the intensity $A^2(t, x)$ can be easily recovered; indeed, at any time $t > 0$, one has

$$A^2(t, x) = A_0^2(y) \left| \frac{\partial y}{\partial x} \right|.$$

One can deduce from (2.6) that $x = y + tu_0(y) = y + tu(t, x)$, so the last expression boils down to

$$\left| \frac{\partial y}{\partial x} \right| = 1 - t \partial_x u(t, x),$$

with $u(t, x)$ supposedly known. However, in the homogeneous case, the most accurate way to derive the intensity follows from

$$\left| \frac{\partial y}{\partial x} \right| = \left| \frac{\partial x}{\partial y} \right|^{-1} = \frac{1}{|1 + tu'_0(y)|},$$

which leads to the expression:

$$A^2(t, x) = \frac{A_0(y)^2}{|1 + tu'_0(y)|}, \quad y = x - tu(t, x). \quad (2.11)$$

This formula will be of constant use in the numerical computations; it is of course equivalent to the one written in (2.5) since $\varphi_0''(y) = u_0'(y)$ and $\rho(t, x) = A^2(t, x)$.

2.4. The ray-tracing method

For the sake of completeness, we shortly recall the ray-tracing method as a numerical tool. It consists in sampling a compact interval of the real axis into a collection of abscissas y_l , $l = 1, 2, \dots$ and then shoot rays forward in time using the equations (2.6). The velocity $u(t, x)$ is found through the conservation law $u(t, x) = u_0(y)$ and the intensity is deduced by means of (2.11). One of its main shortcomings is the loss of accuracy in the rarefaction fans, see Fig.4 in [11] or [2, 9, 29], which imposes repetitive regridding processes.

3. Two numerical strategies based on moments

For purely computational reasons, the simulation of a transport equation of the type (2.8) may be considered as too expensive since the velocity variable ξ would have to be sampled too. So a classical idea to move back to a less big computational space is to take moments in ξ in order to work in the physical space t, x only.

3.1. The Delta-closure (Wigner analysis)

This is the most direct way to proceed; namely, one considers (2.8) and integrate against ξ to derive an infinite hierarchy:

$$\partial_t m_i + \partial_x m_{i+1} = 0, \quad m_i(t, x) = \int_{\mathbb{R}} \xi^{i-1} W(t, x, \xi) . d\xi, \quad i = 1, 2, \dots \quad (3.12)$$

However, it isn't always necessary to simulate such a big system; as an example, if $u'_0(x) \geq 0$, $W(t, x, \xi)$ keeps on being monokinetic and (3.12) reduces to the pressureless gas system, [6],

$$\partial_t \rho + \partial_x q = 0, \quad \partial_t q + \partial_x (q^2 / \rho) = 0, \quad q / \rho = u.$$

In this last case, ρ and u remain smooth. When breakup occurs, for some $t^* \in \mathbb{R}^+$, equations (2.6) admit several roots y_j and a more intricate kinetic density is to be inserted inside (3.12). Following [28, 25, 18, 9, 6], we can assume an upper bound $j \leq K \in \mathbb{N}$ and postulate that

$$W(t, x, \xi) = \sum_{j=1}^K A_j(t, x)^2 \delta(\xi - u_j(t, x)), \quad j = 1, 2, \dots, K.$$

Then one has to consider $2K$ moments in order to close (3.12):

$$\partial_t m_1 + \partial_x m_2 = 0, \quad \partial_t m_2 + \partial_x m_3 = 0, \quad \dots \quad \partial_t m_{2K} + \partial_x m_{2K+1} = 0, \quad (3.13)$$

where $m_i(t, x) = \sum_{j=1}^K \rho_j(t, x) u_j(t, x)^{i-1}$, $i = 1, 2, \dots, 2K$. Closing (3.13) amounts to expressing m_{2K+1} as a function of m_1, m_2, \dots, m_{2K} . Despite the fact it is theoretically doable, it remains a difficult task for $K > 4$. Even worse, systems (3.13)

are generally only **weakly hyperbolic** and admit measure-solutions. This makes numerical simulations delicate; results are available in [3, 9, 13, 18].

3.2. The Heaviside-closure (K-branch solutions)

It has been observed [4] that the geometric solutions of Burgers' equation with $u_0(x) \geq 0$ can be recovered out of a kinetic problem in the flavour of (2.8),

$$\partial_t f + \xi \partial_x f = 0, \quad f(t = 0, x, \xi) = H(u_0(x) - \xi)H(\xi),$$

with H the Heaviside function. Beyond breakup time, f ceases to be of this monokinetic-like form and a correct representation would be,

$$f(t, x, \xi) = \sum_{j=1}^K (-1)^{j-1} H(u_j(t, x) - \xi), \quad (3.14)$$

as long as no more than K folds appear. A remarkable feature is that (3.14) can be obtained from an entropy minimization process; this eventually led to the definition of *K-multivalued solutions* in [5] (the classical entropy solutions [22] correspond to $K = 1$). These K-multivalued solutions admit a kinetic formulation:

Definition 1. *We call K-multivalued solution any measurable function $f(t, x, \xi) \in \{0, 1\}$ on $\mathbb{R} \times \mathbb{R}^+ \times \mathbb{R}^+$ satisfying the following equation in the sense of distributions*

$$\partial_t f + \xi \partial_x f = (-1)^{K-1} \partial_\xi^K \tilde{m}, \quad f(t, x, \xi) = \sum_{j=1}^K (-1)^{j-1} H(u_j(t, x) - \xi), \quad (3.15)$$

where \tilde{m} is a nonnegative Radon measure on $\mathbb{R} \times \mathbb{R}^+ \times \mathbb{R}^+$.

The set of $u_j(t, x)$'s is called the *K-branch entropy solution* of Burgers' equation, [11]. The same way as in the preceding section, one considers moments $m_i(t, x) = \frac{1}{i} \sum_{j=1}^K (-1)^{j-1} u_j(t, x)^{i-1}$, $i = 1, 2, \dots, K$ and an equivalence result holds:

Theorem 3.1. *(Brenier & Corrias, [5])*

A measurable function $f(t, x, \xi) = \sum_{j=1}^K (-1)^{j-1} H(u_j(t, x) - \xi)$ is a K-multivalued solution if and only if all the following entropy inequalities hold for any $\theta, \partial_\xi^K \theta \geq 0$:

$$\partial_t \int_{\mathbb{R}^+} \theta(\xi) f(t, x, \xi) \cdot d\xi + \partial_x \int_{\mathbb{R}^+} \xi \theta(\xi) f(t, x, \xi) \cdot d\xi \leq 0. \quad (3.16)$$

Equality holds in case $\partial_\xi^K \theta \equiv 0$.

A beautiful property is that this construction is consistent with the Delta-closure coming from Wigner analysis:

Theorem 3.2. (Equivalence of moment systems, [13])

Let $0 \leq u_0 = \partial_x \varphi_0$ be a smooth function and $\tilde{w}(t = 0, x, \xi)$ be the solution of

the Liouville equation (2.8) with initial condition, $\tilde{w}(t = 0, x, \xi) = H(u_0(x) - \xi)$. Consider the set:

$$\mathcal{C} = \left\{ \xi \in \mathbb{R}^+ \text{ such that } \tilde{w}(t, x, \xi) = 1, \text{ for some } (t, x) \in \mathbb{R}^+ \times \mathbb{R} \right\}.$$

Assume that \mathcal{C} has only M connected components. If $M = \frac{1}{2}(K + 1)$ (K odd) or $M = K/2$ (K even), then the moment systems (3.13) and (3.16) produce the same velocities $u_j(t, x)$, $j = 1, 2, \dots, K$.

Of course, formula (2.11) is to be used in order to deduce the intensities in a consistent way from the K -branch entropy solution. We close this section mentioning that the choice of the upper bound $K \in \mathbb{N}$ can be done relying on the rigorous results of [30]; see [14].

3.3. About multivalued intensities

As one may be especially interested in recovering physical observables which are single-valued, we want to explain how to work them out of the $u_j(t, x)$'s and the $A_j(t, x)$'s, $j = 1, 2, \dots, K$. For instance, the position density associated to (2.5) is an oscillatory object since cross-terms will exhibit small-scale behaviour. However, following [14], we observe that they can be expected to become negligible as $\varepsilon \rightarrow 0$ relying on a stationary phase argument. Let us pick up a smooth test function $\phi(t, x)$ and consider, for $j, j' \leq K$,

$$\forall t > 0, \quad \int_{\mathbb{R}} A_j(t, x) A_{j'}(t, x) \exp\left(i(\varphi_j - \varphi_{j'})(t, x)/\varepsilon\right) \phi(t, x) dx.$$

Thus the stationary phase lemma ensures that if ϕ is supported in a domain where (A_j, φ_j) and $(A_{j'}, \varphi_{j'})$ are C^∞ , this integral is $O(\varepsilon)$ except on points where $\partial_x(\varphi_j - \varphi_{j'})(t, x) = (u_j - u_{j'})(t, x) = 0$, that is, on caustics.

All in all, we have obtained that a very reasonable approximation of the first quadratic observable for small $\varepsilon \geq 0$ is given by the simple expression:

$$\psi \bar{\psi}(t, x) = |\psi(t, x)|^2 \simeq \sum_{j=1}^K |A_j(t, x)|^2. \quad (3.17)$$

This will be checked numerically in the next section; other quadratic observables could be derived similarly.

4. Numerical results: a Gaussian pulse

We give as an initial data for (1.2)–(1.3) the following WKB pulse:

$$\psi_0(x) = \exp\left(-\frac{1}{2}(x - \pi)^2\right) \cdot \exp(-i \cos(x)/\varepsilon), \quad x \in [0, 2\pi]. \quad (4.18)$$

4.1. K-branch solutions and the corresponding intensity

This corresponds to $\varphi_0(x) = -\cos(x)$, $u_0(x) = \sin(x)$, and $A_0(x) = \exp(-\frac{1}{2}(x - \pi)^2)$ which are all C^∞ . We shall not give details about the numerical schemes we used for simulating the K-branch solutions related to this problem; everything is to be found in [11, 13, 14]. The meshing was $\Delta x = 2\pi/512$, $\Delta t = \Delta x/1.05$ and the solutions are shown in $t = 3$ on Fig.1. The rays can be seen on Fig.2 in [13]; a

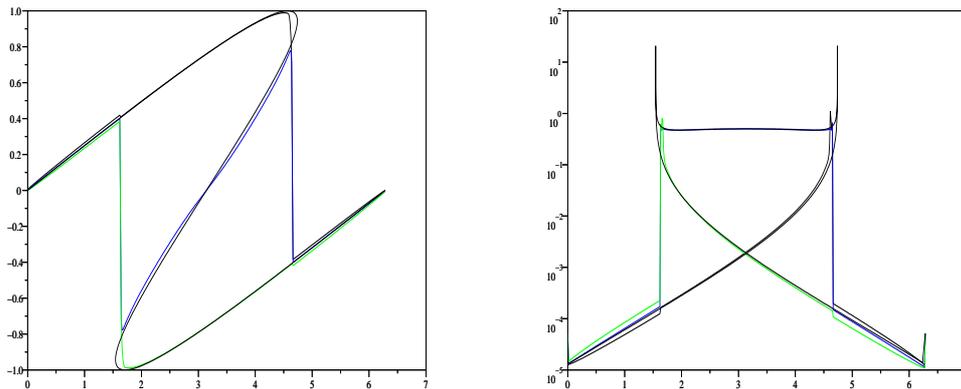


Figure 1: Comparison between the WKB solution and the ray-tracing one in $t = 3$.

so-called cusp singularity develops and the geometric solution of Burgers' equation admits 3 values inside the central fan. The K-branch solution matches the ray-tracing profile with very good accuracy.

4.2. Comparison with the Schrödinger equation

Relying on (3.17), (2.11), we derived the approximate position density we compared with the one coming out of a standard Fourier scheme for (1.2) (see [1]) with 2^{12} modes. One can see the agreement as ε is decreased on Fig.2; the Schrödinger solution's density oscillates at higher and higher frequencies around the value which has been obtained out of the WKB computation. We took $\varepsilon = 1/50, 1/85, 1/145, 1/220$.

5. Conclusion

We tried to give an overview on some efficient computational methods for the semiclassical approximation of (1.2)–(1.3). Apart from stationary phase arguments, we emphasized most of all kinetic-based methods. Two main classes exist nowadays: the one based on Wigner equation (2.8) and the other coming from the K-multibranch solutions of [5]. When it is applicable, the second one leads usually to lighter numerical algorithms. However, open problems subsist: the hardest one being the passage from moments coordinates $m_i(t, x)$ to K-branch solutions $u_j(t, x)$. This is a well-known inverse problem called the **Markov moment problem**; progress are expected to be made in this direction, [15, 27]. Other strategies are available, see [2, 9, 19, 24, 29].

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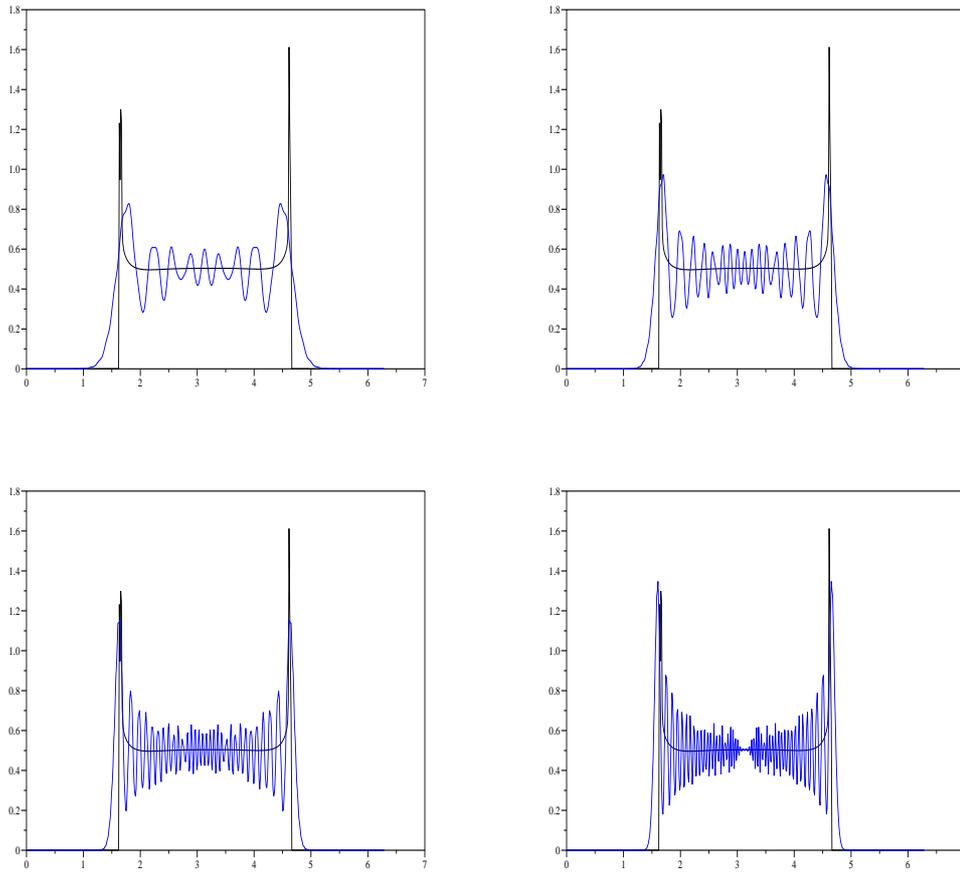


Figure 2: Comparison between the WKB position density (3.17), (2.11), and a direct Schrödinger simulation in $t = 3$.