University of Crete

Department of Mathematics and Applied Mathematics

Diploma Thesis

Quantum Hydrodynamics near caustics

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Abstract

We consider some basic features of quantum hydrodynamics near simple fold and cusp caustics. We show that the initial value problem for the Bohmian trajectories is not well posed, since the quantum potential and the derivatives of the phase of the wave function are too singular. These observations imply, that in the classical limit, the Bohmian trajectories do not converge to the geometric rays because caustics onset at $t = 0+$.

Key Words. quantum hydrodynamics, Bohm equations, Bohm trajectories, geometrical optics, Wigner transform, caustics, Burger's equation, quantum potential.

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Περίληψη

Εξετάζουμε κάποια βασικά χαρακτηριστικά της κβαντικής υδροδυναμικής κοντά στις καυστικές fold και cusp. Επίσης, αποδεικνύουμε ότι το πρόβλημα αρχικών τιμών για τις Bohm τροχιές δεν είναι καλά ορισμένο, αφού το κβαντικό δυναμικό και οι παράγωγοι της φάσης της κυματοσυνάρτησης παρουσιάζουν κάποιες ιδιομορφίες. Αυτές οι παρατηρήσεις, υποδεικνύουν, ότι στο κλασσικό όριο, οι Bohm τροχιές δεν συγκλίνουν στα γεωμετρικά rays, επειδή οι καυστικές ξεκινούν σε χρόνο $t = 0+$.

Λέξεις κλειδιά. κβαντική υδροδυναμική, εξισώσεις Bohm, τροχιές Bohm, γεωμετρική οπτική, μετασχηματισμός Wigner, καυστικές, εξίσωση Burger's, κβαντικό δυναμικό.

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Chapter 1

Introduction

Semiclassical approximations for the Schrödinger equation

$$i\varepsilon\partial_t\psi^\varepsilon(x,t) = \left(-\frac{\varepsilon^2}{2}\partial_x^2 + V(x)\right)\psi^\varepsilon(x,t)\ , \qquad x\in\mathbb{R}, t>0\ ,$$

are important in quantum mechanics [Gr] and high-frequency paraxial wave propagation in inhomogeneous media [Tap]. Traditionally, such approximations have been constructed by the WKB method (or "geometrical optics" method) which is based on the approximation

$$\psi^\varepsilon(\mathbf{x},t) \approx A(x,t)e^{\frac{i}{\varepsilon}\Phi(x,t)}\ ,$$

where the amplitude and the phase satisfy the equations

$$\partial_t\Phi + \frac{1}{2}\big(\partial_x\Phi\big)^2 + V = 0\ ,$$
$$\partial_t A^2 + \partial_x\big(A^2\partial_x\Phi\big) = 0\ .$$

This is a very powerful method not only to draw a qualitative picture of how the energy propagates along the rays, but also to evaluate the wave fields quantitatively. However, WKB approximation fails either on caustics and focal points where it predicts infinite wave amplitudes, or in shadow regions (i.e. regions devoid of rays) where it yields zero fields. On the other hand, formation of caustics is a typical situation in quantum mechanics [BM], [Haa], optics [BU], underwater acoustics [TC] and seismology [Ce], as a result of multiple path propagation.

1.1 Caustics and phase-space methods

Geometrically, caustic surfaces are envelopes of rays. Physically, these surfaces are distinctive in that the field intensity increases on them sharply as compared with the adjacent regions. The rise of field is best of all seen at the focal points where all the rays corresponding to the converging wave front intersect. Moving across a caustic gives birth or annihilation of a pair of rays at a time, and this discontinuous variation of the number of rays across a caustic is qualified as a *catastrophe*. This new and fruitful approach to caustics, developed only in the recent years, allows a universal classification of the typical caustics (see, e.g., [KO]). From specific examples allowing exact solutions, it has been known that the phase of the wave fields change by $-\pi/2$ upon touching a smooth (nonsingular) caustic, and by $-\pi$ after passing a three-dimensional focus. However, a universal rule on the additional phase shift at a caustic has been formulated only in the comparative recent works of Maslov [MA1], [MA2], although the germ of the idea goes back to Keller [KEL]. The formulation is based on the stationary-phase approximation of certain diffraction integrals, and it finally leads to the notion of the so-called KMAH (Keller-Maslov-Arnold-Hormander) index, in the general case of multiple caustic reflections. Because the wave amplitude predicted by geometrical optics is infinite on the caustics, as a result of ray convergence, geometrical optics is inapplicable within a close neighborhood of the caustic, as actual wave fields are always finite. However, available exact and approximate solutions for certain canonical wave problems involving caustics in the high-frequency limit, indicate a substantial concentration of energy near a caustic. This phenomenon is more profound within a finite region which is usually referred as caustic zone or caustic volume. The rigorous estimation of the size of this zone should rely upon delicate uniform asymptotic expansions of certain canonical diffraction integrals associated with the particular caustic, but for the moment only heuristic estimations leading rather to qualitative than to fully quantitative results exist. A very important feature is that the rays cannot be adequately resolved in the caustic zone, and therefore we can draw the general conclusion that within any caustic zone, no physical device is capable of separate determination of ray parameters. In this sense, in that caustic zone, rays loose their physical individual properties, though they continue to play the role of the geometric framework for the wave field.

From the mathematical point of view, formation of caustics and the related multivaluedness of the phase function, is the main obstacle in constructing global high-frequency solutions of the wave equation. The problem of obtaining the multivalued phase function is traditionally handled by resolving numerically the characteristic field related to the eikonal equation (ray tracing methods). Given the geometry of the multivalued phase function, a number of local and uniform methods to describe wave fields near caustics have been proposed. The local methods are essentially based on *boundary layer* techniques as they were developed by Babich, Keller, et.al. (see, e.g., [BAKI], [BB]). The uniform are those which exploit the fact that even if the family of rays has caustics, there are no such singularities for the family of the bicharacteristics in the phase space. This basic fact allows the construction of formal asymptotic solutions (FAS) which are valid also near and on the caustics. For this purpose two main asymptotic techniques have been developed. The first one is the*Kravtsov-Ludwig method* (sometimes called the *method of relevant functions*). This method starts with a modified FAS involving Airy-type integrals, the phase functions of which take account of the particular type of caustics. The second one is the *method of the canonical operator* developed by Maslov. The construction of the canonical operator exploits the fact that the Hamiltonian flow associated with the bicharacteristics generates a Lagrangian submanifold in the phase space, on which we can “lift” the phase function in a unique way [MF].

1.2 The Wigner-function approach

A relatively new technique to treat high frequency dispersive problems is based on the Wigner transform

$$W^{\varepsilon}(x,k,t) = \frac{1}{\pi\varepsilon}\int_{-\infty}^{+\infty} e^{-i\frac{2k}{\varepsilon}\sigma}\psi^{\varepsilon}(x+\sigma,t)\bar{\psi^{\varepsilon}}(x-\sigma,t)d\sigma \ ,$$

whose basic properties (i.e. the relation of its moments with important physical quantities, as energy density, current density, et.al.), make it a proper and extremely useful tool for the study of the wavefield. Wigner function is a phase space object satisfying an integro-differential equation (Wigner equation), which for smooth medium properties can be expressed as an infinite order singular perturbation (with dispersion terms with respect to the momentum of the phase space)of the classical Liouville equation. At the high frequency limit, the solution of the Wigner equation converges weakly to the so called Wigner measure [LP] governed by the classical Liouville equation, and this measure, in general, reproduces the solution of single phase geometrical optics.

We should note at this point that there does not exist, up to now, either some systematic theoretical study of the Wigner integro-differential equation (except the results of Markowich [Mar] for the equivalence of Wigner and Schrödinger equations). This is due to fundamental difficulties of this equation, which is an equation with non-constant coefficients, that combines at least two different characters, that of transport and that of dispersive equations. The first character is correlated with the Hamiltonian system of the Liouville equation (and the classical mechanics of the problem), and the second with the quantum energy transfer away from the Lagrangian manifold of the Hamiltonian system, but mainly inside a boundary layer around it, the width of which depends on the smoothness of the manifold and the presence or not of caustics.

Moreover, in the case of multi-phase optics and caustic formation, Wigner measure is not the appropriate tool for the study of the semi-classical limit. In fact, it has been shown by Filippas & Makrakis [FM] through examples *in the case of time-dependent Schrödinger equation* that the Wigner measure (a) it cannot be expressed as a distribution with respect to the momentum for a fixed space-time point, and thus cannot produce the amplitude of the wavefunction, and (b) it is unable to "recognize" the correct frequency dependencies of the wavefield near caustics. However, it was explained, that the solutions of the integro-differential Wigner equation do have the capability to capture the correct frequency scales. It must be said here, that a numerical approach based on classical Liouville equation has been developed, as an alternative to WKB method, in order to capture the multivalued solutions far from the caustic. This technique is based on a *closure assumption* for a system of equations for the moments of the Wigner measure (essentially by assuming a fixed number of rays passing through a particular point) [JL].

1.3 Bohm equations and Quantum Hydrodynamics

A fluid dynamical formulation of the Schrödinger equation is known since the early years of quantum mechanics. A year after Schrödinger published his celebrated equation, Erwin Madelung showed (in 1927) that it can be written in a hydrodynamic form [Mad]. Madelung's representation has a seemingly major disadvantage by transforming the single linear Schrödinger equation into two nonlinear ones. Nonetheless, despite of its additional complexity, the hydrodynamic analogy provides important insights with regard to the Schrödinger equation. The Madelung equations (ME) describe a compressible fluid, and compressibility yields a linkage between hydrodynamic and thermodynamic effects. A simple derivation uses the polar decomposition of the wave function

$$\psi^{\varepsilon}(x,t) = \mathrm{R}^{\varepsilon}(x,t)e^{\frac{i}{\varepsilon}\mathrm{S}^{\varepsilon}(x,t)} \ .$$

Separating the real and the imaginary part of the single-state Schrödinger equation gives the system of Bohm equations

$$\partial_t \mathrm{S}^\varepsilon + \frac{1}{2}\big(\partial_x \mathrm{S}^\varepsilon\big)^2 + V + Q^\varepsilon = 0 \ ,$$
$$\partial_t \big(\mathrm{R}^\varepsilon\big)^2 + \partial_x \cdot \Big(\big(\mathrm{R}^\varepsilon\big)^2 \partial_x \mathrm{S}^\varepsilon\Big) = 0 \ ,$$

where Q^ε is the quantum potential

$$Q^\varepsilon = -\frac{\varepsilon^2}{2}\frac{\partial_x^2 \mathrm{R}^\varepsilon}{\mathrm{R}^\varepsilon} \ ,$$

which is a nonlocal perturbation of the external potential V and, formally, it vanishes in the classical limit.

The hydrodynamic formulation follows by considering a "quantum fluid" that has density $\rho^\varepsilon = |\mathrm{R}^\varepsilon|^2$ and moves with Eulerian velocity $\mathrm{z}^\varepsilon = \partial_x \mathrm{S}^\varepsilon$. It turns out that the motion of the fluid satisfies the Euler equations

$$\partial_t \rho^\varepsilon + \partial_x(\rho^\varepsilon \mathrm{z}^\varepsilon) = 0 \ ,$$
$$\rho^\varepsilon(\partial_t \mathrm{z}^\varepsilon + \mathrm{z}^\varepsilon \partial_x \mathrm{z}^\varepsilon) = -\partial_x p^\varepsilon + \rho^\varepsilon b^\varepsilon \ ,$$

with pressure $p^\varepsilon = -\frac{\varepsilon^2}{4}\rho^\varepsilon \partial_x^2 \rho^\varepsilon$ and body force $b^\varepsilon = -\frac{\partial_x V}{\rho^\varepsilon}$.

Moreover, it turns out that z^ε satisfies the inhomogeneous Burgers equation

$$\partial_t z^\varepsilon + z^\varepsilon \partial_x z^\varepsilon = -\partial_x(Q^\varepsilon + V) \ .$$

In Bohmian mechanics a particle is not simply described by its wave function ψ^ε as in the standard interpretation of quantum mechanics. Rather, the wave function, called by de Broglie the pilot-wave [Bro], drives the motion of the particle and it is used to compute the velocity (or momentum) of the particle, whose dynamics is consequently given by the characteristics of the Burgers equation.

The above description of the particle's dynamics can be considered as the Eulerian approach to Bohmian mechanics since z^ε is the associated Eulerian velocity. While it is certainly interesting to directly study their limits as $\varepsilon \to 0$, this problem seems to be out of reach so far and hence will not be the object of this paper. Instead, Markowich and his collaborators [MPS1], [MPS2] have described how to pass to the corresponding Lagrangian point of view of Bohmain dynamics and argued that this viewpoint naturally leads to the introduction of a certain class of probability measures on phase space, which they call Bohmian measures. These measures concentrate on Lagrangian sub-manifolds in phase space induced by the graph of the initial velocity $\psi^\varepsilon(x, 0)$. They consequently proceeded via the (Lagrangian version of the) Bohmian dynamics and they showed to be equivariant with respect to this phase space flow. Moreover they showed that before the onset of caustics, the Bohmian trajectories converge to the rays of geometrical optics.

In this work, we compute the quantum potential in certain simple examples where caustics onset at $t = 0+$, and we show that, in this case, Bohmian trajectories cannot be defined because someone cannot compute initial data for the Burgers equation. This observation implies the conjecture that Bohmian mechanics does not converge to classical mechanics after caustics onset.

Chapter 2

Geometrical optics-WKB method, caustics

In this chapter we are concerned with the *Wentzel-Kramers-Brillouin* (WKB) method, which shows the correspondence between classical and quantum mechanics by considering the behavior of the wave function $\psi^{\varepsilon}(\mathbf{x},t)$, and also provides useful approximations to the solutions of the Schrödinger equation describing the state of a non-relativistic quantum particle. [MG] The WKB method, also known as WKB approximation, is a semiclassical calculation in quantum mechanics, based on the exponential function which is semiclassically expanded, and then either the amplitude or the phase is taken to be slowly varying.

We consider the Cauchy problem for the time-dependent one-dimensional Schrödinger equation with fast temporal and spatial scales, and highly oscillatory initial data

$$\begin{cases} i\varepsilon\partial_t\psi^{\varepsilon}(x,t) = \left(-\frac{\varepsilon^2}{2}\partial_x^2 + V(x)\right)\psi^{\varepsilon}(x,t), & x\in\mathbb{R}\ ,\ t>0\ , \\ \psi^{\varepsilon}(x,0) = \psi_0^{\varepsilon}(x) = A_0(x)e^{\frac{i}{\varepsilon}\mathrm{S}_0(x)} & x\in\mathbb{R}\ , \end{cases} \tag{2.1}$$

where i is the imaginary unit, ε is the semiclassical parameter (scaled Planck constant), $V(x)$ is its potential energy, and ψ^{ε} is the wave function (more precisely, in this context, it is called the "position-space wave function"). The operator $\left(-\frac{\varepsilon^2}{2}\partial_x^2 + V(x)\right)$ is the quantization of the Hamiltonian function, that is the total energy, equals kinetic energy plus potential energy, of the corresponding classical particle.

Moreover, the parameter ε respesents the space-time scales, as well as the typical wave length of oscillations of the initial data.

We are interested in the high-frequency solution of (2.1), that is the expansion of ψ^{ε} in the regime $\varepsilon \ll 1$, which will be referred to as the the *semi-classical limit*. The limit case when we consider that $\varepsilon \to 0$ will be referred to as the the *classical limit* (or the *geometrical-optics solution*). The mode of transition form the semiclassical regime to the classical limit. It is a very delicate problem because the Schrödinger equation propagates oscillations of wave lengths ε which inhibit ψ^{ε} from converging strongly in a suitable sense.

2.1 The WKB ansatz

In order to apply the *geometrical optics technique* [BLP, Ra], one seeks for an approximating WKB solution of the form

$$\psi^\varepsilon(x,t) = A^\varepsilon(x,t)e^{\frac{i}{\varepsilon}\Phi^\varepsilon(x,t)} \ , \tag{2.2}$$

where the amplitude A^ε and the phase Φ^ε, are real valued functions, and they admit of the regular perturbation expansions

$$A^\varepsilon(x,t) = A(x,t) + \varepsilon A_1(x,t) + \varepsilon^2 A_2(x,t) + \ldots\ldots \tag{2.3}$$

and

$$\Phi^\varepsilon(x,t) = \Phi(x,t) + \varepsilon\Phi_1(x,t) + \varepsilon^2\Phi_2(x,t) + \ldots\ldots \tag{2.4}$$

Then, the derivatives of the wave function are given by

$$\partial_t\psi^\varepsilon = \Big(\partial_t A^\varepsilon + \frac{i}{\varepsilon}A^\varepsilon\partial_t\Phi^\varepsilon\Big)e^{\frac{i}{\varepsilon}\Phi^\varepsilon}, \tag{2.5}$$

$$\partial_x\psi^\varepsilon = \Big(\partial_x A^\varepsilon + \frac{i}{\varepsilon}A^\varepsilon\partial_x\Phi^\varepsilon\Big)e^{\frac{i}{\varepsilon}\Phi^\varepsilon}, \tag{2.6}$$

$$\partial_x\psi^\varepsilon = \partial_x\big(\partial_x\psi^\varepsilon\big) = \Big(\partial_x A^\varepsilon - \frac{1}{\varepsilon^2}A^\varepsilon\big(\partial_x\Phi^\varepsilon\big)^2 + \frac{1}{\varepsilon}\big(A^\varepsilon\partial_x^2\Phi^\varepsilon + 2\partial_x\Phi^\varepsilon\partial_x A^\varepsilon\big)\Big)e^{\frac{i}{\varepsilon}\Phi^\varepsilon} \ . \tag{2.7}$$

By substituting (2.5) , (2.6) , (2.7) into (2.1) we rewrite the Schrödinger equation in the form

$$i\varepsilon\big(\partial_t A^\varepsilon + \frac{i}{\varepsilon}A^\varepsilon\partial_t\Phi^\varepsilon\big) = -\frac{\varepsilon^2}{2}\Big(\partial_x A^\varepsilon - \frac{1}{\varepsilon^2}A^\varepsilon\big(\partial_x\Phi^\varepsilon\big)^2 + \frac{1}{\varepsilon}\big(A^\varepsilon\partial_x\Phi^\varepsilon + 2\partial_x\Phi^\varepsilon\partial_x A^\varepsilon\big)\Big) + VA^\varepsilon \ . \tag{2.8}$$

We further substitute the expansions (2.3) , (2.4) into (2.8), and we get the asymptotic equation

$$\varepsilon^0 A\bigg(\partial_t\Phi + \frac{1}{2}\big(\partial_x\Phi\big)^2 + V\bigg) - i\varepsilon\bigg(\partial_t A + \frac{1}{2}\big(A\partial_x^2\Phi + 2\partial_x\Phi\partial_x A\big)\bigg) - \frac{\varepsilon^2}{2}\partial_x^2 A + \cdots = 0 \ . \tag{2.9}$$

If we assume that A , Φ are smooth functions, equation (2.9) is satisfied to order $O(\varepsilon^2)$, if the phase Φ satisfies the *Hamilton-Jacobi equation*

$$\partial_t\Phi + \frac{1}{2}\big(\partial_x\Phi\big)^2 + V = 0 \ , \tag{2.10}$$

and the amplitude A satisfies the *transport equation*

$$\partial_t A^2 + \partial_x\big(A^2\partial_x\Phi\big) = 0 \ . \tag{2.11}$$

Remark. The equations (2.10) , (2.11) are the fundamental equations of *geometrical optics*, and they define the principal term $\psi^\varepsilon(\mathbf{x},t) \approx A(x,t)e^{\frac{i}{\varepsilon}\Phi(x,t)}$ in the asymptotic expansion of the wave function. It is remarkable that the Hamilton-Jacobi equation for the phase Φ is the same with the equation governing the phase in classical mechanics, while the transport equation for the amplitude A expresses the conservation of particles moving under the action of the potential V. These two facts, express the well-known analogy between classical mechanics and geometrical optics (see, e.g., [Gold], [Arn]).

2.2 Hamiltonian system and rays

The Hamilton-Jabobi and the transport equations are partial differential equations of the first order, and their solution can be constructed by reduction to ordinary differential equations along the rays as follows [Ev]. Let

$$H(x,k)=\frac{1}{2}k^2+V(x)\ , \tag{2.12}$$

be the Hamiltonian function. We consider the *Hamiltonian system* [BLP]

$$\begin{cases} \frac{dx(t;q,p)}{dt}=k(t;q,p)\ , \\ \frac{dk(t;q,p)}{dt}=-V'\big(x(t;q,p)\big)\ , \\ x(0;q,p)=q, \qquad k(0;q,p)=p\ . \end{cases} \tag{2.13}$$

The trajectories of this system are the *bicharacteristics* in the phase space $\mathbb{R}^2_{xk}$. When the initial momentum is given by $p=\mathrm{S}_0'(q)$, then, the projections of the bicharacteristics on to the $\mathbb{R}^2_{xt}$ space are the *rays* of geometrical optics. In order to distinguish between the rays and the bicharacteristics we denote the rays by $\bar{x}=\bar{x}(t;q)$, and it turns out that they are solutions of the system

$$\begin{cases} \frac{d\bar{x}(t;q)}{dt}=\bar{k}(t;q)\ , \\ \frac{d\bar{k}(t;q)}{dt}=-V'\big(\bar{x}(t;q)\big)\ , \\ \bar{x}(0;q)=q\ , \quad \bar{k}(0;q)=\mathrm{S}_0'(q)\ . \end{cases} \tag{2.14}$$

Therefore the rays are the projections on to the physical space of the bicharacteristics emanating from the initial Lagrangian manifold (curve) $\Lambda_0=\{(q,p)|p=\mathrm{S}_0'(q)\}$ in phase space.

Note that for the free Schrödinger equation, that is $V(x)=0$, the rays are given by

$$\begin{cases} \bar{x}(t;q)=\mathrm{S}_0'(q)t+q\ , \\ \bar{k}(t;q)=\bar{k}(0;q)=\mathrm{S}_0'(q)\ , \end{cases} \tag{2.15}$$

that is, they are the straight lines in the space-time $\mathbb{R}^2_{xt}$ emanating at $(x=q\ ,t=0)$ with constant slope $\mathrm{S}_0'(q)$.

The Jacobian of the ray transformation $q\mapsto\bar{x}(t;q)$ is given by

$$\mathrm{J}(t;q)=\frac{\partial\bar{x}(t;q)}{\partial q}\ . \tag{2.16}$$

Whenever the Jacobian (2.16) vanishes, the ray transformation is multi-valued, and a caustic appears. Near the caustic the rays may cross and have other complicated singularities. The singularities depend on the particular form of the initial data. If $t=t_c(q)$ are the solutions of the equation $\mathrm{J}(t;q) = 0$, then the caustic has the parametric equations

$$\begin{cases} t = t_c(q) \ , \\ \bar{x}_c(q) = \bar{x}\big(t_c(q);q\big) \ . \end{cases} \tag{2.17}$$

2.3 Integration of Hamilton-Jacobi equation

By the identification $k = \partial_x \Phi(x,t)$, the initial value problem for the Hamilton-Jacobi equation (2.10) is written in the form

$$\begin{cases} \partial_t \Phi(x,t) + H(x, \partial_x \Phi(x,t)) = 0 \ , & x \in \mathbb{R}, t > 0 \ , \\ \Phi(x, t=0) = \mathrm{S}_0(x) \ . & x \in \mathbb{R} \ . \end{cases} \tag{2.18}$$

This form of the Hamilton-Jacobi equation, suggests that the equation can be reduced to an ordinary differential equation along the rays (see, [Ev], Sec. 3.2.5 , 3.3.1 for a rigorous explanation). In fact, by differentiating along the ray $\bar{x} = \bar{x}(t;q)$, and using the equations (2.14), we have

$$\begin{aligned} \frac{d}{dt}\Phi\big(\bar{x}(t;q),t\big) &= \partial_t \Phi\big(\bar{x}(t;q),t\big) + \partial_x \Phi\big(\bar{x}(t;q),t\big)\frac{d\bar{x}(t;q)}{dt} \\ &= -\left(\frac{1}{2}\Big(\partial_x\Phi\big(\bar{x}(t;q),t\big)\Big)^2 + V\big(\bar{x}(t,q)\big)\right) + \partial_x\Phi\big(\bar{x}(t;q),t\big)\bar{k}(t;q) \\ &= -\frac{1}{2}\bar{k}^2(t;q) - V\big(\bar{x}(t;q)\big) + \bar{k}^2(t;q) \\ &= \frac{1}{2}\bar{k}^2(t;q) - V\big(\bar{x}(t;q)\big) \ . \end{aligned} \tag{2.19}$$

We integrate (2.19) on the internal $(0,t)$, we immediately derive the phase

$$\Phi(\bar{x},t) = \mathrm{S}_0(q) + \int_0^t \left(\frac{1}{2}\bar{k}^2(\tau;q) - V\Big(\bar{x}(\tau;q)\Big)\right)d\tau \ . \tag{2.20}$$

2.4 Integration of the transport equation

We solve now the initial value problem for the transport equation

$$\begin{cases} \partial_t \mathrm{A}^2(x,t) + \partial_x\big(\mathrm{A}^2(x,t)\partial_x\Phi(x,t)\big) = 0, \quad x \in \mathbb{R}, \ t > 0 \ , \\ \mathrm{A}(x,t=0) = \mathrm{A}_0(x) \ , \ x \in \mathbb{R} \ . \end{cases} \tag{2.21}$$

First, we differentiate lnA^2 along the rays, and we get

$$\begin{aligned}\frac{d}{dt}\ln \mathrm{A}^2\big(\bar{x}(t,\alpha),t\big) &= \frac{1}{\mathrm{A}^2\big(\bar{x}(t,\alpha),t\big)}\frac{d}{dt}\mathrm{A}^2\big(\bar{x}(t,\alpha),t\big)\\ &= \frac{\big(\partial_t \mathrm{A}^2+\partial_x \mathrm{A}^2\partial_x\Phi\big)\big(\bar{x}(t,\alpha),t\big)}{\mathrm{A}^2\big(\bar{x}(t,\alpha),t\big)}\\ &= -\partial_x^2\Phi\big(\bar{x}(t,\alpha),t\big)\ .\end{aligned} \tag{2.22}$$

Then, by Liouville's formula (see Appendix 1) for the equation

$$\frac{d\bar{x}}{dt} = \bar{k} = \partial_x\Phi\big(\bar{x}(t,q)\ ,$$

we get

$$\frac{d}{dt}\ln \mathrm{J}(t,q) = \partial_x\bar{k}(t,q) = \partial_x\Big(\partial_x\Phi\big(\bar{x}(t,q),t\big)\Big) = \partial_x^2\Phi\big(\bar{x}(t,q),t\big)\ . \tag{2.23}$$

Thus, we obtain

$$\frac{d}{dt}\ln \mathrm{A}^2\big(\bar{x}(t,\alpha),t\big) = -\frac{d}{dt}\ln \mathrm{J}(t,q)\ . \tag{2.24}$$

Finally, by assuming that $\mathrm{J}(t,q)\neq 0$ on the internal $(0,t)$, we integrate the last equation, and we derive

$$\mathrm{A}\big(\bar{x}(t,q),t\big) = \frac{\mathrm{A}_0(q)}{\sqrt{\mathrm{J}(t,q)}}\ . \tag{2.25}$$

Remark. Note that $\mathrm{J}(t=0,q)=1$, since for $t=0$, the ray map is the identity, and $\mathrm{J}(t,q)>0$ as long as caustics do not appear. However, for the critical caustic time $t=t_c(q)$, the Jacobian vanishes and the geometrical amplitude (2.25) becomes infinite on the caustic. Therefore, when caustics appear the WKB method fails to predict the amplitude of the wave function, and other techniques must be applied (see, e.g., [FM] for a concise review of such methods).

Chapter 3

Quantum Hydrodynamics

3.1 Bohm equations and quantum potential

In order to motivate the introduction of the particle concept into quantum mechanics, Erwin Madelung decomposed the Schrödinger equation into two real equations, in a particular way, by expressing the complex-valued time-dependent wave function in polar form

$$\psi^\varepsilon(x,t) = \mathrm{R}^\varepsilon(x,t) e^{\frac{i}{\varepsilon}\mathrm{S}^\varepsilon(x,t)} \ , \tag{3.1}$$

where

$$\mathrm{R}^\varepsilon(x,t) = |\psi^\varepsilon(x,t)|^2 \tag{3.2}$$

is the amplitude and

$$\mathrm{S}^\varepsilon(x,t) = \varepsilon \arg \psi^\varepsilon \tag{3.3}$$

is the phase of the wavefunction, both depending of ε.

Substituting (3.1) into the Schrödinger equation (2.1) we obtain

$$i\varepsilon\big(\partial_t \mathrm{R}^\varepsilon + \frac{i}{\varepsilon}\mathrm{R}^\varepsilon \partial_t \mathrm{S}^\varepsilon\big) = -\frac{\varepsilon^2}{2}\Big[\partial_x^2 \mathrm{R}^\varepsilon - \frac{1}{\varepsilon^2}\mathrm{R}^\varepsilon\big(\partial_x \mathrm{S}^\varepsilon\big)^2 + \frac{1}{\varepsilon}\big(\mathrm{R}^\varepsilon \partial_x^2 \mathrm{S}^\varepsilon + 2\partial_x \mathrm{S}^\varepsilon \partial_x \mathrm{R}^\varepsilon\big)\Big] + V\mathrm{R}^\varepsilon.$$

Then, seperating into real and imaginary parts yields respectively the following equations

$$-\mathrm{R}^\varepsilon \partial_t \mathrm{S}^\varepsilon = \frac{1}{2}\mathrm{R}^\varepsilon\big(\mathrm{S}^\varepsilon\big)^2 - \frac{\varepsilon^2}{2}\partial_x^2 \mathrm{R}^\varepsilon + V\mathrm{R}^\varepsilon \ , \tag{3.4}$$

and

$$\partial_t \mathrm{R}^\varepsilon = -\frac{1}{2}\big(\mathrm{R}^\varepsilon \partial_x^2 \mathrm{S}^\varepsilon + 2\partial_x \mathrm{S}^\varepsilon \partial_x \mathrm{R}^\varepsilon\big) \ , \tag{3.5}$$

respectively. Assuming that $\mathrm{R}^\varepsilon \neq 0$ we get the equations

$$\partial_t \mathrm{S}^\varepsilon + \frac{1}{2}\big(\partial_x \mathrm{S}^\varepsilon\big)^2 + V + Q^\varepsilon = 0 \ , \tag{3.6}$$

$$\partial_t\big(\mathrm{R}^\varepsilon\big)^2 + \partial_x \cdot \Big(\big(\mathrm{R}^\varepsilon\big)^2 \partial_x \mathrm{S}^\varepsilon\Big) = 0 \ , \tag{3.7}$$

where we have defined the *quantum potential* Q^ε as:

$$Q^\varepsilon = -\frac{\varepsilon^2}{2}\frac{\partial_x^2 \mathrm{R}^\varepsilon}{\mathrm{R}^\varepsilon} \ . \tag{3.8}$$

The initial data for (2.1) imply the initial data

$$\mathrm{R}_0^\varepsilon(x) = \mathrm{R}^\varepsilon(x,0) \equiv A_0(x) \ , \qquad \mathrm{S}_0^\varepsilon(x) = \mathrm{S}^\varepsilon(x,0) \equiv S_0(x) \ . \tag{3.9}$$

The system (3.7), (3.6) is usually referred to as the *Bohm equations* or *the equations of quantum hydrodynamics*, and they form the basis of the so called Bohmian mechanics. By their derivation, these equations are equivalent to the Schrödinger equation. However, they have used as the basis for various approaches in quantum mechanics, as hidden variable theory [B] and de Broglie's pilot wave theory [Hol], [DT], but also for computational purposes in quantum chemistry [Wy].

Although the quantum potential formally appears in the equation (3.6) that suggests a dynamical origin, a closer examination reveals a conceptual structure that is radically different from that used in classical physics. For example, it carries nonlocal features which seem to be essential for a proper description of some quantum effects and it appears to have no well-defined source, so that its interpretation as a dynamical field is inappropriate. Bohm [B] originally considered this to be a weakness of the model and thought it was a temporary feature of the unrefined theory. No doubt, it is the nondynamical nature of the quantum potential that has generated a different attitude.

It is interesting to observe, that from the definition (3.8) of the quantum potential, it follows that the amplitude R^ε satisfies the equation

$$\frac{\varepsilon^2}{2}\frac{\partial^2 \mathrm{R}^\varepsilon}{\partial x^2} + Q^\varepsilon(x,t)\mathrm{R}^\varepsilon = 0 \ . \tag{3.10}$$

The character of this equation may change from elliptic to hyperbolic since the quantum potential changes sign. See, e.g., [Car1], [Car2] for various mathematical aspects of this equation and the role of quantum potential. We must also note that, at least qualitatively, the behaviour of the equation can be related to the properties of the geometrical optics' rays and the behaviour of the WKB solution.

We rewrite Q^ε as follows

$$\begin{aligned}
Q^\varepsilon = \frac{\mathrm{R}^\varepsilon \partial_x^2 \mathrm{R}^\varepsilon}{(\mathrm{R}^\varepsilon)^2} &= -\frac{\varepsilon^2}{2}\frac{\partial_x(\mathrm{R}^\varepsilon\partial_x \mathrm{R}^\varepsilon) - (\partial_x \mathrm{R}^\varepsilon)^2}{(\mathrm{R}^\varepsilon)^2} \\
&= -\frac{\varepsilon^2}{2}\frac{1}{2}\frac{\partial_x^2(\mathrm{R}^\varepsilon)^2 - (\partial_x \mathrm{R}^\varepsilon)^2}{(\mathrm{R}^\varepsilon)^2} \\
&= -\frac{\varepsilon^2}{2}\left(\frac{1}{2}\frac{\partial_x^2(\mathrm{R}^\varepsilon)^2}{(\mathrm{R}^\varepsilon)^2} - \left(\partial_x ln(\mathrm{R}^\varepsilon)\right)^2\right) \\
&= -\frac{\varepsilon^2}{2}\left(\frac{1}{2}\frac{\partial_x^2(\mathrm{R}^\varepsilon)^2}{(\mathrm{R}^\varepsilon)^2} - \left(\partial_x \frac{1}{2} ln(\mathrm{R}^\varepsilon)^2\right)^2\right) \ .
\end{aligned}$$

Thus, the quantum potential is expressed in terms of the energy density

$$\eta^\varepsilon = (\mathrm{R}^\varepsilon)^2 \ , \tag{3.11}$$

in the form

$$Q^\varepsilon(x,t) = -\frac{\varepsilon^2}{2}\left(\frac{1}{2}\frac{\partial_x^2 \eta^\varepsilon}{\eta^\varepsilon} - \left(\frac{1}{2}\partial_x \ln \eta^\varepsilon\right)^2\right) \ . \tag{3.12}$$

3.2 Hydrodynamic variables and the role of quantum potential

We recall now that Euler equations

$$\partial_t \rho + \partial_x(\rho u) = 0 \quad (\text{ conservation of mass}) \ , \tag{3.13}$$

$$\rho(\partial_t u + u\partial_x u) = -\partial_x p + \rho b, \quad (\text{ conservation of momentum}) \ , \tag{3.14}$$

where ρ is the density, u is the Eulerian velocity, p is the pressure and b is the acceleration due to body forces.

We consider now a fluid with density

$$\rho^\varepsilon = \eta^\varepsilon = (\mathrm{R}^\varepsilon)^2, \tag{3.15}$$

and Eulerian velocity

$$z^\varepsilon = \partial_x \mathrm{S}^\varepsilon \ . \tag{3.16}$$

For brevity, we refer to this fluid as the *quantum fluid*, but someone should be very careful to avoid confusion with real fluids where quantum effects are important for the flow. Then, the transport equation (3.7) is written in the form

$$\partial_t \rho^\varepsilon + \partial_x(\rho^\varepsilon z^\varepsilon) = 0 \ , \tag{3.17}$$

By the identification

$$\rho = \rho^\varepsilon \ , \quad u = z^\varepsilon \ , \tag{3.18}$$

we see that equation (3.17) coincides with the continuity equation (3.13).

Furthermore, by differentiating (3.6) with respect to x, and using the definition (3.16) of the fluid velocity, we derive the following inhomogeneous Burgers equation for the velocity

$$\frac{dz^\varepsilon}{dt} = \partial_t z^\varepsilon + z^\varepsilon \partial_x z^\varepsilon = -\partial_x(Q^\varepsilon + V) \ . \tag{3.19}$$

We again use the identification (3.18) and we compare (3.19) with (3.14). It turns out that the pressure p^ε of the quantum fluid must satisfy

$$\partial_x p^\varepsilon = \eta^\varepsilon \partial_x Q^\varepsilon \ , \tag{3.20}$$

and $b^\varepsilon = -\frac{\partial_x V}{\eta^\varepsilon}$. We rewrite the quantum potential (3.12) in the form

$$Q^\varepsilon = -\frac{\varepsilon^2}{4}\left(\frac{1}{2}(\partial_x ln\eta^\varepsilon)^2 + \partial_x^2 ln\eta^\varepsilon\right) \ , \tag{3.21}$$

we differentiate the last equation with respect to x, and we compare the resulting equation with (3.20). It follows that the quantum pressure is given by the formula

$$p^\varepsilon = -\frac{\varepsilon^2}{4}\eta^\varepsilon \partial_x^2 \eta^\varepsilon = -\frac{\varepsilon^2}{4}\rho^\varepsilon \partial_x^2 \rho^\varepsilon \ . \tag{3.22}$$

The quantum pressure depends explicitly on the amplitude $\eta^\varepsilon = (\mathrm{R}^\varepsilon)^2$ and only implicitly on the phase S^ε.

The above explained analogy of quantum mechanics hydrodynamics (hence the term *quantum hydrodynamics*) was introduced first by Madelung [Mad], and its consequences to quantum theory has been exploited by de Broglie (pilot wave theory) [Bro] and Bohm ("hidden variables" interpretation)[B]. See also [DT] for a detailed mathematical exposition of Bohmian mechanics and quantum potentials, and [Wy] for an exposition of quantum hydrodynamics from the point of view of quantum chemistry.

3.3 Bohm trajectories

The characteristics of this equation

$$\frac{dz^\varepsilon}{dt} = \partial_t z^\varepsilon + z^\varepsilon \partial_x z^\varepsilon = -\partial_x Q^\varepsilon \ , \tag{3.23}$$

are the so called *Bohmian trajectories.* They satisfy the system

$$\begin{cases} \frac{dx^\varepsilon(t;q,p)}{dt} = k^\varepsilon(t;q,p) \ , \\ \\ \frac{dk^\varepsilon(t;q,p)}{dt} = -\partial_x Q^\varepsilon\big(x^\varepsilon(t;q,p),t\big) \ , \\ \\ x^\varepsilon(0;q) = q, \qquad k^\varepsilon(0;q) = z^\varepsilon(q,0) = S_0'(q) \ . \end{cases} \tag{3.24}$$

When the ray field is smooth and there are no caustics, it has been shown the Bohm trajectories exist globally in time [TT], and they converge to the rays as $\varepsilon \to 0$, and the solution of the Burgers equation (3.23) to converge to the derivative of the solution of the Hamilton-Jacobi equation (2.10) [FKMS], [MPS1], [MPS2] (see also [Bo] for the physical content of this convergence). However, this convergence cannot be proved when caustics have been appeared and as we will shown by specific examples in the next chapter even the Bohmian trajectories may be not well defined.

Chapter 4

Quantum potential near caustics

In this chapter, we study a couple of examples in order to get a sense how quantum hydrodynamics works near caustics, and what kind of difficulties someone can face. More precisely, we evaluate the quantum potential and the Bohm trajectories near a fold and the potential near a cusp. For this we need to compute the energy density $\eta^\varepsilon(x,t) = (\mathrm{R}^\varepsilon(x,t))^2$ and the gradient of the phase $\mathrm{z}^\varepsilon(x,t) = \partial_x \mathrm{S}^\varepsilon(x,t)$ of the wave function $\psi^\varepsilon(x,t) = \mathrm{R}^\varepsilon(x,t)e^{\frac{i}{\varepsilon}\mathrm{S}^\varepsilon(x,t)}$. Uniform approximations of η^ε near fold and cusp caustics have been constructed in [FM], by using the Wigner transform. The same method provides z^ε through the energy flux $\mathscr{F}^\varepsilon(x,t) = \frac{\varepsilon}{2i}\big(\bar{\psi}^\varepsilon \partial_x \psi^\varepsilon - \psi^\varepsilon \partial_x \bar{\psi}^\varepsilon\big)$.

The Wigner transform of the wavefunction $\psi^\varepsilon(x,t)$ is defined by

$$W^\varepsilon(x,k,t) = W^\varepsilon[\psi^\varepsilon](x,k,t) = \frac{1}{\pi\varepsilon}\int_{-\infty}^{+\infty} e^{-i\frac{2k}{\varepsilon}\sigma}\psi^\varepsilon(x+\sigma,t)\bar{\psi}^\varepsilon(x-\sigma,t)d\sigma \ . \tag{4.1}$$

In the case of free Schrödinger equation $V(x)\equiv 0$, W^ε satisfies the Liouville equation

$$\partial_t W^\varepsilon + k\partial_x W^\varepsilon = 0 \ , \quad W^\varepsilon(x,k,t=0) = W_0^\varepsilon(q,p) \ , \tag{4.2}$$

where

$$W_0^\varepsilon(q,p) \equiv W^\varepsilon[\psi_0^\varepsilon](q,p) = \frac{1}{\pi\varepsilon}\int_{-\infty}^{+\infty} e^{-i\frac{2p}{\varepsilon}\sigma}\psi_0^\varepsilon(q+\sigma)\bar{\psi}_0^\varepsilon(q-\sigma)d\sigma \ , \tag{4.3}$$

is the Wigner transform of the initial wave function ψ_0^ε.

Then, since, for $V\equiv 0$, the solution of the Hamiltonian system (2.12) is given by

$$\begin{cases} x = pt + q \ , \\ k = p \ , \end{cases} \tag{4.4}$$

the elementary transport equation (4.2) has the solution

$$W^\varepsilon(x,k,t) = W_0^\varepsilon(x-kt,k) \ , \tag{4.5}$$

By integration of the Wigner function, it follows that

$$\eta^\varepsilon(x,t) = |\psi^\varepsilon|^2 = \int_{-\infty}^{+\infty} W^\varepsilon(x,k,t)dk \ ,$$

and

$$\mathscr{F}^\varepsilon(x,t) = \frac{\varepsilon}{2i}\big(\bar{\psi}^\varepsilon \partial_x \psi^\varepsilon - \psi^\varepsilon \partial_x \bar{\psi}^\varepsilon\big) = (\mathrm{R}^\varepsilon)^2 \partial_x \mathrm{S}^\varepsilon = \int_{\mathbb{R}} k W^\varepsilon(x,k,t)dk \ .$$

Therefore

$$(\mathrm{R}^\varepsilon(x,t))^2 = \int_{-\infty}^{+\infty} W^\varepsilon(x,k,t)dk \ , \tag{4.6}$$

$$\mathrm{z}^\varepsilon(x,t) = \partial_x \mathrm{S}^\varepsilon(x,t) = \frac{1}{(\mathrm{R}^\varepsilon(x,t))^2}\int_{\mathbb{R}} k W^\varepsilon(x,k,t)dk \ . \tag{4.7}$$

4.1 Example 1: Focal point

4.1.1 Rays and caustic

Recall that we deal only with the free Schrödinger equation, that is $V(x) \equiv 0$. First, we construct the WKB with initial data

$$A_0(q) \equiv 1 \ , \qquad \mathrm{S}_0(q) = -\frac{q^2}{2} \ . \tag{4.8}$$

In this case, the rays are emanating from the solution of the system (2.15) and they have the form

$$\bar{x}(t;r) = r(1-t) \ . \tag{4.9}$$

Also, the momentum is given by

$$\bar{k}(t;r) = \bar{k}(0;q) = \mathrm{S}_0'(r) = -r \ . \tag{4.10}$$

According to the equation (2.16) the Jacobian is $J(t;r) = 1-t$ and vanishes at time $t_c = 1$. Therefore, the caustic is the focal point

$$t = t_c = 1 \ , \quad x = x_c = \bar{x}(t_c(r);r) = 0 \ , \ \text{for any } r \ ,$$

and we observe that for $t = 1$, all rays pass through the focal point. However, there is not a shadow zone.

4.1.2 Calculation of $\eta^\varepsilon = (\mathrm{R}^\varepsilon)^2$

The Wigner transform of the initial wave function is given by substituting the initial wave function $\psi_0^\varepsilon(q) = e^{-\frac{i}{\varepsilon}\frac{q^2}{2}}$ into (4.3),

$$W_0^\varepsilon(q,p) := W^\varepsilon[\psi_0^\varepsilon](q,p) = \frac{1}{\pi\varepsilon}\int_{-\infty}^{+\infty} e^{\left(i\frac{2(p+q)}{\varepsilon}\sigma\right)} d\sigma = \delta(p+q) \ , \tag{4.11}$$

where $\delta(x)$ is the Dirac's delta function. Then, by (4.5) we find

$$W^\varepsilon(x,k,t) = \delta(k + (x-kt)) = |\frac{1}{t-1}|\delta\big(k - \frac{x}{t-1}\big) \ . \tag{4.12}$$

We proceed now to calculate the amplitude R^{ε} by using equation (4.6). We have

$$(\mathrm{R}^{\varepsilon}(x,t))^2 = \left|\frac{1}{t-1}\right| . \tag{4.13}$$

The amplitude satisfies the correct initial data $(\mathrm{R}^{\varepsilon}(q,0))^2 = 1 = A_0^2(q)$. By the definition (3.8) of the quantum potential it follows that $Q^{\varepsilon}(x,t) = 0$ for all $x \in \mathbb{R}, \ , t > 0$, and therefore the Bohmian trajectories coincide with the rays.

4.1.3 Calculation of $\mathrm{z}^{\varepsilon} = \partial_x \mathrm{S}^{\varepsilon}$

We proceed to calculate z^{ε} by substituting (4.25) and (4.12) into (4.7). We easily derive

$$\mathrm{z}^{\varepsilon}(x,t) = \frac{x}{t-1} , \tag{4.14}$$

and it is easy to check that z^{ε} satisfies the homogeneous Burgers equation (3.19) since Q^{ε} and V vanish identically. Also, it satisfies the correct initial data $\mathrm{z}^{\varepsilon}(q,0) = -q = \mathrm{S}'{}_0(q)$.

Remark. Similar results are derived for the initial phase $\mathrm{S}_0(q) = +\frac{q^2}{2}$, by formally substituting $(t+1)$ in place of $(t-1)$ in the above formulas for J and z^{ε}. In this case, the rays diverge and there is not any focal point $\big($the focal point is moved to the non physical point $(x=0 \ , t=-1)\big)$.

In the following examples, we will see that in the case of fold and cusp caustics that both the amplitude and the derivative of the phase do not satisfy the initial data and the corresponding problems for the Burgers equation and the Bohmian trajectories are not well posed.

4.2 Example 2: Fold

4.2.1 Rays and caustic

Recall that we deal only with the free Schrödinger equation, that is $V(x) \equiv 0$. First, we construct the WKB with initial data

$$A_0(q) \equiv 1 , \qquad \mathrm{S}_0(q) = -\frac{q^3}{3} . \tag{4.15}$$

In this case, the rays are given by the solution of the system

$$\begin{cases} \frac{d\bar{x}(t;r)}{dt} = \bar{k}(t;r) , \\ \frac{d\bar{k}(t;r)}{dt} = 0 , \\ \bar{x}(0;r) = r , \qquad \bar{k}(0;r) = \mathrm{S}_0'(r) = -r^2 . \end{cases} \tag{4.16}$$

Obviously, the momentum is given by

$$\bar{k}(t;r) = \bar{k}(0;r) = \mathrm{S}_0'(r) = -r^2 ,$$

and the rays are the straight lines

$$\bar{x}(t;r) = \mathrm{S}_0'(r)t + r = -r^2 t + r \ . \tag{4.17}$$

By (2.16), the Jacobian is given by

$$J(t;r) = \frac{\partial \bar{x}(t;r)}{\partial r} = -2rt + 1 = 0 \ . \tag{4.18}$$

Eliminating the initial position r from the equations (4.17), (4.18), we find that the caustic is the hyperbola $xt = \frac{1}{4}$ in space-time $\mathbb{R}^2_{xt}$.

In order to describe the geometry of the rays near the caustics, we argue as follows. From the ray equation (4.17) we have $tr^2 - r + \bar{x} = 0$. The discriminant $\Delta = 1 - 4\bar{x}t$ of this equation vanishes on the caustic, and it has two real roots $r_{1,2} = r_{\pm}(\bar{x}, t) = \frac{1 \mp \sqrt{1-4\bar{x}t}}{2t}$ in the illuminated zone $4\bar{x}t \leq 1$. This means that, from each point $(\bar{x}, t)$ in the illuminated zone pass two rays, which emanate from the points $r_{1,2}$ on the $x-$ axis. On the other hand, there are not any rays that penetrate the shadow zone $4\bar{x}t > 1$. Such an arrangement of rays characterises the caustics as fold.

By the equations (2.25), (2.20), we find that the amplitudes and the phases along the rays in the illuminated zone are given by

$$A_{\pm}^2(\bar{x}, t) = \frac{A_0^2\big(q(\bar{x}, t)\big)}{J_{\pm}(t; r_{\pm})} = \frac{1}{\pm\sqrt{1 - 4\bar{x}t}} \ . \tag{4.19}$$

and

$$\partial_x \Phi_{\pm}(x, t) = \frac{-1 + 2xt \pm \sqrt{1 - 4xt}}{2t^2}. \tag{4.20}$$

where the indices $\pm$ correspond to the rays emanating from the initial positions $\pm r$.

The amplitude along the ray emanating from r_- is obviously complex. This means that the wave associated with this ray suffers a phase jump equals to $\frac{\pi}{2}$, when the rays touches the fold.

4.2.2 Calculation of $\eta^\varepsilon = (\mathrm{R}^\varepsilon)^2$

The Wigner transform of the initial wave function is given by substituting the initial wave function $\psi_0^\varepsilon(q) = e^{\frac{i}{\varepsilon}\frac{q^3}{3}}$ into (4.3),

$$W_0^\varepsilon(q, p) := W^\varepsilon[\psi_0^\varepsilon](q, p) = \frac{1}{\pi\varepsilon} \int_{-\infty}^{+\infty} e^{\left[-i\left(\frac{2}{3\varepsilon}\sigma^3 + \frac{2}{\varepsilon}(p+q^2)\sigma\right)\right]} d\sigma \ , \tag{4.21}$$

and it is expressed explicitly in terms of the Airy function

$$W^\varepsilon[\psi_0^\varepsilon](q, p) = \frac{2^{\frac{2}{3}}}{\varepsilon^{\frac{2}{3}}} Ai\left(\frac{2^{\frac{2}{3}}(p + q^2)}{\varepsilon^{\frac{2}{3}}}\right) \ . \tag{4.22}$$

Then, by (4.5) we find

$$W^\varepsilon(x, k, t) = \frac{2^{\frac{2}{3}}}{\varepsilon^{\frac{2}{3}}} Ai\left(\frac{2^{\frac{2}{3}}\left(k^2t^2 + (1 - 2xt)k + x^2\right)}{\varepsilon^{\frac{2}{3}}}\right) \ . \tag{4.23}$$

It can be shown that as $\varepsilon \to 0$, W^ε trends to a Dirac function "concentrated" on the Lagrangian manifold (parabola) $\Lambda_t = \{(x,k) : k^2t^2 + (1-2xt)k + x^2 = 0\}$. We observe that for any $t > 0$, in opposite to the single-phase optics, Λ_t is no longer the graph of a single-valued function $k = \Phi_x(x,t)$. Instead, it consists of two single (real-valued) branches $k = \Phi_x^+(x,t)$ and $k = \Phi_x^-(x,t)$, which exist only in the illuminated zone ($xt < \frac{1}{4}$) Thus, W^ε can be written as

$$W^\varepsilon(x,k,t) = \frac{2^{\frac{2}{3}}}{\varepsilon^{\frac{2}{3}}} Ai\left(\frac{2^{\frac{2}{3}}}{\varepsilon^{\frac{2}{3}}} t^2 \big(k - \Phi_x^-(x,t)\big)\big(k - \Phi_x^+(x,t)\big) \right) . \tag{4.24}$$

On the caustic $x_f = \frac{1}{4t}$, we observe that $\Phi_x^+(x_f,t) = \Phi_x^-(x_f,t) = -\frac{1}{4t^2} \equiv k_f$, and the expression defining Λ_t becomes a perfect square in k, which is the typical behavior of Lagrangian manifolds near folds. Clearly, at these points, $\frac{dx}{dk} = 0$ and the manifold Λ_t turns vertically.

We proceed now to calculate the amplitude R^ε by using equation (4.6). This calculation can be explicitly computed by means of the following "projection identity",

$$\int_{-\infty}^{+\infty} Ai(\alpha k^2 + bk + c)dk = \frac{2\pi}{2^{\frac{1}{3}}\sqrt{\alpha}} Ai^2\left(-\frac{b^2 - 4ac}{4^{\frac{5}{3}}\alpha} \right), \quad \alpha > 0 \ .$$

with $\alpha = \left(\frac{2}{\varepsilon}\right)^{\frac{2}{3}} t^2$, $\quad b = \left(\frac{2}{\varepsilon}\right)^{\frac{2}{3}}(1-2xt)$, $\quad c = \left(\frac{2}{\varepsilon}\right)^{\frac{2}{3}} x^2$, and it leads to

$$(\mathrm{R}^\varepsilon(x,t))^2 = \frac{2\pi}{\varepsilon^{\frac{1}{3}} t} Ai^2\left(-\frac{1}{\varepsilon^{\frac{2}{3}} t^2} \frac{1-4xt}{4} \right), \quad t > 0 \ . \tag{4.25}$$

We note that in the illuminated zone $xt < \frac{1}{4}$, the argument of $Ai^2(\cdot)$ is negative, and therefore, as $\varepsilon \to 0$, R^ε is rapidly oscillating away from the caustic, while in the shadow zone the argument of $Ai^2(\cdot)$ is positive and R^ε is exponentially decreasing. This picture is qualitatively and quantitatively compatible with the predictions of the WKB solution.

4.2.3 Calculation of $\mathrm{z}^\varepsilon = \partial_x \mathrm{S}^\varepsilon$

We proceed to calculate z^ε by substituting (4.25) and (4.24) into (4.7).

The computation of the energy flux, and other higher order moments of the Wigner function has been done in [KM], and it is based on the integration formula [VS]

$$\int_{-\infty}^{+\infty} Ai(u^2 - \lambda)u^m du = (-1)^m i^m \left(\frac{\partial^m \mathrm{F}(\lambda,\xi)}{\partial \xi^m} \right)_{\xi=0}, \tag{4.26}$$

where

$$\mathrm{F}(\lambda,\xi) = \int_{-\infty}^{+\infty} e^{i\xi u} Ai(u^2 - \lambda)du = 2^{\frac{2}{3}}\pi Ai\big(-2^{-\frac{2}{3}}(\lambda+\xi)\big) Ai\big(-2^{-\frac{2}{3}}(\lambda-\xi)\big) \ . \tag{4.27}$$

By these results, we derive

$$\mathrm{z}^\varepsilon(x,t) = \frac{2xt - 1}{2t^2} \ , \tag{4.28}$$

and it is easy to check that z^ε satisfies the Burgers equation (3.19).

4.2.4 Calculation of Quantum Potential

We proceed to the calculation of quantum potential, by using (3.12) with (eq. (4.25))

$$\eta^{\varepsilon} = (\mathrm{R}^{\varepsilon})^2 = \frac{2\pi}{\varepsilon^{\frac{1}{3}} t} Ai^2\Big(-\frac{1}{\varepsilon^{\frac{2}{3}} t^2} \frac{1-4xt}{4} \Big) \ .$$

We set

$$\omega = -\frac{1}{\varepsilon^{\frac{2}{3}} t^2} \frac{1-4xt}{4} \ .$$

The first derivative of η^{ε} with respect to x is

$$\frac{\partial \eta^{\varepsilon}}{\partial x} = \frac{4\pi}{\varepsilon t^2} Ai(\omega) Ai'(\omega) \ . \tag{4.29}$$

We differentiate the last equation again with respect to x, and using the Airy differential equation $Ai''(u) - uAi(u) = 0$, we get

$$\frac{\partial^2 \eta^{\varepsilon}}{\partial x^2} = \frac{4\pi}{\varepsilon^{\frac{5}{3}} t^3} \Big(\big(Ai'(\omega)\big)^2 + uAi^2(\omega) \Big) \ . \tag{4.30}$$

By substituting (4.29), (4.30) into the definition of the quantum potential (eq. (3.8)), we have

$$\begin{aligned} Q^{\varepsilon} &= -\frac{\varepsilon^2}{4} \frac{1}{\frac{2\pi}{e^{\frac{1}{3}} t} Ai^2(\omega)} \left(\frac{\partial^2 \eta^{\varepsilon}}{\partial_x^2} \right) + \frac{\varepsilon^2}{8} \frac{1}{\frac{4\pi^2}{\varepsilon^{\frac{2}{3}} t^2} Ai^4(\omega)} \left(\frac{\partial \eta^{\varepsilon}}{\partial x} \right)^2 \\ &= -\frac{\varepsilon^{\frac{2}{3}}}{2t^2} \left[\frac{\big(Ai'(\omega)\big)^2}{Ai^2(\omega)} + \omega \right] + \frac{\varepsilon^{\frac{2}{3}}}{2t^2} \frac{\big(Ai'(\omega)\big)^2}{Ai^2(\omega)} = -\frac{\varepsilon^{\frac{2}{3}}}{2t^2} \omega \ . \end{aligned}$$

Thus, the quantum potential for our particular problem is given by the simple formula

$$Q^{\varepsilon} = \frac{1-4xt}{8t^4} \ . \tag{4.31}$$

We observe that Q^{ε} is independent of ε, and therefore it does not vanish when $\varepsilon \to 0$ as someone might expect to happen (compare with the case of the cusp in Example 3 in the next section). Moreover, it is zero on the fold, and it is positive in the illuminated zone. Then, equation (3.10) shows that the amplitude is rapidly oscillating away from the caustic in the illuminated zone.

4.2.5 The Bohmian trajectories

We observe that (4.28), (4.31) satisfy the Burgers equation (3.23). However, z^{ε} is not defined for $t = 0$ (actually it goes to infinity), and it is therefore impossible to prescribe initial data for the Burgers equation. The same difficulty arises in solving the system (3.24) for the Bohmian trajectories, because (4.28) is incompatible with the initial data $k^{\varepsilon}(0; q) = z^{\varepsilon}(q, 0) = S_0'(q) = -q^2$. Therefore, it seems that it is impossible to solve the initial value problems for the Burgers equation and for the Bohmian trajectories. We think that this difficulty comes from the fact that the caustics onsets at $t = 0$.

In order to exploit the structure of the Bohmian trajectories, we will consider three particular cases. The general form of the trajectories is (actually they are independent of ε since the quantum potential is independent of ε in this case)

$$x^{\varepsilon}(t;\alpha\ ,\beta) = \frac{1}{4t} + \alpha t + \beta\ , \quad k^{\varepsilon}(t;\alpha) = -\frac{1}{4t^2} + \alpha\ . \tag{4.32}$$

Case 1: Since $k^{\varepsilon} = \mathrm{z}^{\varepsilon}(x,t) = \frac{2xt-1}{2t^2} = 0$ on the curve $(x = q\ ,\ t = \frac{1}{2q})\ , q > 0$, we easily find that the trajectories passing from these points are given by

$$x^{\varepsilon}(t;q) = \frac{1}{4t} + q^2 t\ , \quad k^{\varepsilon}(t;q) = -\frac{1}{4t^2} + q^2\ . \tag{4.33}$$

It is easy to check that they remain in the shadow zone for all time.

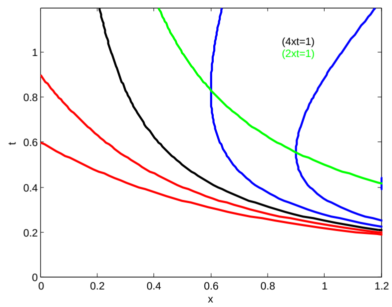

Figure 4.1: *Bohmian trajectories near the fold.*

Case 2: If we consider the trajectories passing from the points $(x = q\ ,\ t = \frac{1}{4q})\ , q > 0$ which are on the caustic, we find

$$x^{\varepsilon}(t;q) = \frac{1}{4t}\ , \quad k^{\varepsilon}(t;q) = -\frac{1}{4t^2}\ . \tag{4.34}$$

Consequently, these particular trajectories remain on the caustic for all time.

Case 3: In order to exploit the trajectories in the illuminated zone, we consider the trajectories passing from the points $(x=0\ ,t=\tau)\ ,\tau>0$. These trajectories are given by

$$x^{\varepsilon}(t;q)=\frac{1}{4t}-\frac{t}{4\tau^2}\ ,\quad k^{\varepsilon}(t;q)=-\frac{1}{4t^2}-\frac{1}{4\tau^2}\ . \tag{4.35}$$

It is easy to check that they remain in the illuminated zone for all time.

In all cases, the trajectories move out towards $x=+\infty$ as $t\to 0+$ approaching indefinitely the caustic, and they never cross.

4.3 Example 3: Cusp

In this case, we calculate only the quantum potential, but we do not derive z^{ε} and we do not deal with the Bohmian trajectories. An analysis similar to that we did for the fold is in principle possible, but the completion of the calculations requires much more effort and time because they involve the Pearcey integral, and it goes beyond the scope of an undergraduate diploma thesis.

4.3.1 Rays and caustic

Now we construct the WKB of the free Schrödinger equation with initial data

$$\mathrm{A}_0\equiv 1\ ,\quad \mathrm{S}_0(q)=-\frac{q^4}{4}-\alpha q^2+bq,\quad \alpha>0,\quad b>0\ . \tag{4.36}$$

In this case the rays are deare given by the system

$$\begin{cases}\frac{d\bar{x}(t;r)}{dt}=\bar{k}(t;r)\ ,\\ \frac{d\bar{k}(t;r)}{dt}=0\ ,\\ \bar{x}(0;r)=r\ ,\qquad \bar{k}(0;r)=\mathrm{S}_0'(r)=-r^2\ .\end{cases} \tag{4.37}$$

Obviously the momentum is given by $\bar{k}(t;r)=\bar{k}(0;r)=\mathrm{S}_0'(r)=-r^3-2\alpha r+b,\quad \alpha\ ,b>0$, and the rays are the straight lines

$$\bar{x}(t;r)=\mathrm{S}_0'(r)t+r=-r^3t+(1-2\alpha t)r+bt\ . \tag{4.38}$$

By (2.16), the caustic is given by

$$J(t;r)=\frac{\partial\bar{x}(t;r)}{\partial r}=-3r^2t+1-2\alpha t=0\ . \tag{4.39}$$

Eliminating the initial position r from the equations (4.38), (4.39), we find that the caustic is given by the cusp curve

$$27u^2=4v^3\ ,\quad u=\frac{x}{t}-b,\quad v=\frac{1}{t}-2\alpha\ . \tag{4.40}$$

The beak of the cusp is the point $u=v=0$, that is $\left(x_b=\frac{b}{2\alpha},t_b=\frac{1}{2\alpha}\right)$.

4.3.2 Calculation of R^ε

The Wigner transform of the initial wave function is calculated by substituting the initial wave function $\psi_0^\varepsilon(q) = e^{\frac{i}{\varepsilon}(-\frac{q^4}{4}-\alpha q^2+bq)}$ into (4.3), and using the integral representation of the Airy function. For $q \neq 0$ we get

$$W^\varepsilon[\psi_0^\varepsilon](q,p) = \left(\frac{2}{\varepsilon}\right)^{\frac{2}{3}} \frac{1}{|3q|^{\frac{1}{3}}} Ai\left(\frac{2^{\frac{2}{3}}(q^3+2\alpha q+p-b)}{\varepsilon^{\frac{2}{3}}(3q)^{\frac{1}{3}}}\right) , \tag{4.41a}$$

while for $q = 0$ we get a Dirac mass,

$$W^\varepsilon[\psi_0^\varepsilon](q,p) = \delta(p-b) \ . \tag{4.41b}$$

Although $q = 0$ is a singular point of the initial Wigner function $W_0^\varepsilon(q,p)$, using the distributional formula

$$\frac{1}{\epsilon} Ai\left(\frac{y}{\epsilon}\right) \to \delta(y) \ , \quad \epsilon \to 0 \ ,$$

we see that

$$W_0^\varepsilon(q,p) \to W_0^\varepsilon(0,p), \qquad q \to 0 \ .$$

Then, by (4.5) we find

$$W^\varepsilon(x,k,t) = W_0^\varepsilon(x-kt,k) = \begin{cases} \left(\frac{2}{\varepsilon}\right)^{\frac{2}{3}} \frac{1}{|3(x-kt)|^{\frac{1}{3}}} Ai\left(\frac{2^{\frac{2}{3}}\left[(x-kt)^3+2\alpha(x-kt)+k-b\right]}{\varepsilon^{\frac{2}{3}}\left[3(x-kt)\right]^{\frac{1}{3}}}\right), & x \neq kt, \\ \delta(k-b), & x = kt. \end{cases} \tag{4.42}$$

As $\varepsilon \to 0$, we see that W^ε is an Airy function "concentrated" on the Lagrangian manifold

$$\Lambda_t = \{(x,k) : k^3t^3 - 3xt^2k^2 - (1-3tx^2-2\alpha t)k - x^3 - 2\alpha x + b = 0)\}.$$

We note that for $0 < t < \frac{1}{2\alpha}$, there is a region $\big(x_1(t) < x < x_2(t)\big)$ where this manifold consists of three branches. Notice that points $x_1(t)$ and $x_2(t)$ trace the fold sides of the cusp. At $t = \frac{1}{2\alpha}$, this region degenerates to the point $B = \big(x = \frac{b}{2\alpha}, k = b\big)$ which is an inflection point of Λ_t with vertical tangent. Point B projects onto the beak of the cusp. For $t > \frac{1}{2\alpha}$ the manifold becomes and stays thereafter single-valued.

We proceed now to calculate the amplitude R^ε by using equation (4.6). This calculation can be explicitly computed by means of the following "projection identity" [FM]

$$\int_{-\infty}^{+\infty} \frac{1}{|\xi|^{\frac{1}{3}}} Ai\left(\frac{\lambda}{\xi^{\frac{1}{3}}}(\xi^3 - v\xi + u)\right) d\xi = \frac{3^{\frac{1}{4}}}{2\pi\sqrt{2}\lambda^{\frac{1}{4}}} |P(V,U)|^2, \qquad \lambda > 0 \ , \tag{4.43}$$

where $P(V,U)$ denotes the Pearcey integral [Kam], [Wo]

$$P(V,U) = \int_{\mathbb{R}} e^{\left[i\left(\frac{t^4}{4}+V\frac{t^2}{2}+Ut\right)\right]} dt \ , \tag{4.44}$$

with

$$V = -\frac{1}{\sqrt{2}}\lambda^{\frac{3}{4}}3^{\frac{1}{4}}v \ , \qquad U = \frac{1}{2^{\frac{3}{4}}}\lambda^{\frac{9}{8}}3^{\frac{3}{8}}u \ .$$

Thus, we obtain

$$(\mathrm{R}^{\varepsilon}(x,t))^2 = \frac{1}{2\pi t}\left(\frac{2}{\varepsilon}\right)^{\frac{1}{2}} |P(r,s)|^2 \ , \tag{4.45}$$

where

$$r = -\frac{1}{\varepsilon^{\frac{1}{2}}} v \ , \qquad s = \frac{1}{\varepsilon^{\frac{3}{4}}} u \ . \tag{4.46}$$

and

$$u = \frac{x}{t} - b \ , \qquad v = \frac{1}{t} - 2\alpha \ . \tag{4.47}$$

Calculation of quantum potential

We proceed to calculate the quantum potential by (3.12). First we compute the derivatives

$$\partial_x |P(r,s)|^2 = 2Re(\bar{P}\partial_x P) \ , \qquad \partial_x^2 |P(r,s)|^2 = 2Re(\bar{P}\partial_x^2 P) + 2|\partial_x P|^2$$

and

$$\partial_x P(r,s) = \frac{1}{\varepsilon^{\frac{3}{4}} t} \partial_s P(r,s) \ , \qquad \partial_x^2 P(r,s) = \frac{1}{\varepsilon^{\frac{3}{2}} t^2} \partial_s^2 P(r,s)$$

we get

$$\partial_x \eta^{\varepsilon} = \frac{1}{\pi t^2} \frac{2^{\frac{1}{2}}}{\varepsilon^{\frac{5}{4}}} Re(\bar{P}\partial_s P) \ , \tag{4.48}$$

$$\partial_x^2 \eta^{\varepsilon} = \frac{2^{\frac{1}{2}}}{\pi t^3 \varepsilon^2} \left(Re(\bar{P}\partial_s^2 P) + |\partial_s P|^2 \right) \ . \tag{4.49}$$

Thus, we write the quantum potential in the form

$$Q^{\varepsilon}(x,t) = \frac{1}{2\varepsilon^{\frac{3}{2}} t^2} \frac{|P|^2 \partial_s^2 |P|^2 - \frac{1}{2}(\partial_s |P|^2)^2}{|P|^4} \ . \tag{4.50}$$

Now, we introduce the new variables

$$r = -\xi \ , \qquad s = \mu \xi^{\frac{3}{2}} \ , \tag{4.51}$$

and we rewrite the Pearcey integral $P(r,s)$ in the form

$$P(r,s) = Y(\xi,\mu) := \int_{-\infty}^{+\infty} e^{i\left(\frac{t^4}{4} - \xi\frac{t^2}{2} + \mu\xi^{\frac{3}{2}} t\right)} dt \ . \tag{4.52}$$

Note that by eliminating ξ in (4.51), and using the (4.47), we get $u^2 = \mu^2 v^3$. For $\mu = \frac{2}{\sqrt{27}}$, the last equation represents the cusp in the caustic coordinates $(u\ ,v)$.

In new variables we have

$$\frac{\partial |P|^2}{\partial s} = \frac{2}{3\mu^{\frac{2}{3}}} s^{-\frac{1}{3}} \frac{\partial}{\partial \xi} |Y|^2 \ , \qquad \frac{\partial^2 |P|^2}{\partial s^2} = \frac{4}{9\mu^{\frac{4}{3}}} s^{-\frac{2}{3}} \frac{\partial^2}{\partial \xi^2} |Y|^2 \ . \tag{4.53}$$

Unfortunately, we cannot proceed in a way similar to that we followed for the fold and we are not able to derive a closed form of the quantum potential. The difficulty comes from the fact that we do not have appropriate differential equations governing the Pearcey integral in order to eliminate the denominator in (4.50). Thus, we are obliged to derive an asymptotic expansion of Q^ε.

For this purpose, we employ the uniform asymptotic expansion [Kam]

$$Y(\xi,\mu) = exp\left(\tfrac{i\xi^2}{2}\left(f(t_2;\mu)+f(t_3;\mu)\right)\right)$$
$$\times\left[p_0(\nu)\tfrac{2\pi}{\xi^{\frac{1}{6}}}Ai\big(-\xi^{\frac{4}{3}}\zeta\big)\left(1+O\left(\tfrac{1}{\xi^2}\right)\right)+q_0(\nu)\tfrac{2\pi}{i\xi^{\frac{5}{6}}}Ai'\big(-\xi^{\frac{4}{3}}\zeta\big)\left(1+O\left(\tfrac{1}{\xi^2}\right)\right)\right]+$$
$$+e^{i\xi^2 f(t_1;\mu)}\left(\tfrac{\pi}{3t_1^2-1}\right)^{\frac{1}{2}}\tfrac{1+i}{\xi^{1/2}}\left(1+O\left(\tfrac{1}{\xi^2}\right)\right),\quad \xi\to\infty\ ,\quad 0\le\mu\le\tfrac{2}{\sqrt{27}}\ , \tag{4.54}$$

where

$$f(t;\mu) = \frac{t^4}{4} - \frac{t^2}{2} + \mu t\ ,$$

and

$$t_1 = -\frac{2}{\sqrt{3}}\sin(\frac{\pi}{3}+\sigma)\ , \qquad t_2 = \frac{2}{\sqrt{3}}\sin\sigma\ , \qquad t_3 = \frac{2}{\sqrt{3}}\sin(\frac{\pi}{3}-\sigma)\ ,$$

with

$$3\sigma = \arcsin\left(1-\frac{\sqrt{27}}{2}\nu\right)\ , \qquad \nu = \frac{2}{\sqrt{27}}-\mu\ ,$$

are the roots of the cubic equation $\partial_t f(t;\mu)=0$.

Note that the uniformity parameter μ, measures the “distance” from the cusp, and the expansion is valid even for $\mu = \frac{2}{\sqrt{27}}$.

The functions p_0 and q_0 are defined by the formulas

$$p_0(\sigma) = \frac{1}{2}\left(\sqrt{\frac{2\zeta^{1/2}}{2\sqrt{3}z_3+3z_3^2}}+\sqrt{\frac{-2\zeta^{1/2}}{2\sqrt{3}z_2+3z_2^2}}\right)\ ,$$

and

$$q_0(\sigma) = \frac{1}{2\zeta^{\frac{1}{2}}}\left(\sqrt{\frac{2\zeta^{1/2}}{2\sqrt{3}z_3+3z_3^2}}-\sqrt{\frac{-2\zeta^{1/2}}{2\sqrt{3}z_2+3z_2^2}}\right)\ ,$$

where $z_1(\sigma), z_2(\sigma), z_3(\sigma)$ are given by

$$z_1(\sigma) = -\frac{2}{\sqrt{3}}\sin\left(\psi+\frac{\pi}{3}\right)-\frac{1}{\sqrt{3}}\ , \qquad z_2(\sigma) = \frac{2}{\sqrt{3}}\sin\psi-\frac{1}{\sqrt{3}}\ ,$$

$$z_3(\sigma) = \frac{2}{\sqrt{3}}\sin\left(\frac{\pi}{3}-\psi\right)-\frac{1}{\sqrt{3}}\ , \qquad 3\psi = \arcsin\left(1-\frac{\sigma\sqrt{27}}{2}\right),\quad |\psi|\le\frac{\pi}{6}\ .$$

The quantities $z_i, i=1,2,3$ are the roots of $\partial_z g(z;s)=0$ with

$$g(z;s) = -\sigma z + \frac{z^3}{\sqrt{3}} + \frac{z^4}{4}\ ,$$

and

$$\zeta^{\frac{3}{2}}(\sigma) = \frac{3}{4}\Big(g(z_2;\sigma)-g(z_3;\sigma)\Big)\ .$$

We observe that $\zeta = 0$ when $z_2 = z_3$ which happens on the cusp.

We combine (4.50), (4.53), (4.54), and after some cumbersome asymptotic algebra, we obtain the expansion

$$Q^{\varepsilon}(x,t) = -\frac{32}{81}\zeta^3\varepsilon^{1/2} + O(\varepsilon^{3/2}) \ , \quad \varepsilon \ll 1 \ , \tag{4.55}$$

We observe that the quantum potential goes to zero as $\varepsilon \to 0$, and that it vanishes on the cusp, since $\zeta(\sigma = \frac{2}{\sqrt{27}})$ vanishes on the cusp. This asymptotic behaviour is completely different than the behaviour of the quantum potential near the fold. We may conjecture that the difference comes from the fact that in the case of the cusp we do not have a shadow zone. On the other hand, preliminary calculations show that the momentum is again too singular at $t = 0+$ and the initial value problem for the Bohmian trajectories is not compatible. These observations imply that although the quantum potential vanishes at the classical limit, the Bohmian trajectories do not converge to the geometrical rays.

Chapter 5

Discussion

We have studied the quantum hydrodynamics for the free Schrödinger near three elementary caustics: the focal point, the fold and the cusp. We have shown that in the case of the focal point the Bohmian trajectories coincide with the geometric rays, since the quantum potential is identically zero. In the case of the fold, we found that the quantum potential is independent of the semiclassical parameter ε and it vanishes on the caustic. We have faced a major difficulty: the Bohmian trajectories and the corresponding Burgers equation fail to satisfy the initial data since the caustics onsets at $t = 0+$ at infinity. In order to identify the origin of this difficulty, we employed the Wigner transform in order to compute the derivative of the phase of the wave function and to trace the Bohmian trajectories. It turned out, that the trajectories never cross and trajectories starting on the caustic remain on the caustic forever. In the case of the cusp, the quantum potential depends on the semiclassical parameter and we have only calculated the main asymptotic term in its expansion for small ε. The approximate potential vanishes on the cusp. Preliminary calculations imply that higher order terms also vanish on the caustic, and that the initial value problem for the Bohmian trajectories is not well posed in this case too. The tracing of Bohmian trajectories is open interesting question, because in the case of the cusp there is not a shadow zone (but only a less illuminated single-phase zone), and we would like to understand how Bohmian trajectories escape from the beak of the caustic.

Appendix A

The Liouville formula

Lemma A.0.1. [Har] Consider the autonomous system of n equations

$$\frac{dx(t)}{dt} = f(x), \qquad x \in \mathbb{R}^n \tag{A.1}$$

with $f(x) \in \mathrm{C}^\infty(\mathbb{R}^n_x)$. Let $x(t,q) \in \mathrm{C}^\infty\big(\mathrm{I} \times \mathrm{V}\big)$, an $(n-1)$-parameter family of solutions, $\alpha = (\alpha_1, \ldots, \alpha_{n-1}) \in \mathbb{R}^{n-1}_\alpha$, $\mathrm{V} \subseteq \mathbb{R}^{n-1}_\alpha$, $\quad \mathrm{I} = \{|t| < \delta\}$ for some $\delta > 0$. Set

$$\mathrm{J}(t,\alpha) = \det \frac{\partial_x(t,\alpha)}{\partial(t,\alpha)} \ , \tag{A.2}$$

and assume that $\mathrm{J}(t,\alpha) \neq 0$ for $(t,\alpha) \in \big(\mathrm{I} \times \mathrm{V}\big)$. Then the Liouville formula

$$\frac{d}{dt} \ln \mathrm{J}(t,\alpha) = \mathrm{tr}\Big(\nabla_x f\big(x(t,\alpha)\big)\Big) = \nabla_x \cdot f\big(x(t,\alpha)\big) \ , \tag{A.3}$$

holds for $(t,\alpha) \in \big(\mathrm{I} \times \mathrm{V}\big)$.

Proof. For matrix $\mathrm{A}(t) \in \mathrm{C}^1(\mathrm{I})$, $\quad \det \mathrm{A}(t) \neq 0, \quad t \in \mathrm{I},$ the Jacobi formula

$$\frac{d}{dt} \ln \big(\det \mathrm{A}(t)\big) = \mathrm{tr}\Big(\mathrm{A}^{-1}(t) \frac{d\mathrm{A}(t)}{dt}\Big) \ , \tag{A.4}$$

holds: From (2.22) we have

$$\begin{aligned} \frac{dx(t,\alpha)}{dt} &= f\big(x(t,\alpha)\big) \implies \\ \frac{\partial}{\partial t}\Big(\frac{\partial_x(t,\alpha)}{\partial(t,\alpha)}\Big) &= \nabla_x f\big(x(t,\alpha)\big) \frac{\partial_x(t,\alpha)}{\partial(t,\alpha)} \ . \end{aligned} \tag{A.5}$$

We apply formula (2.25) with $\mathrm{A} = \frac{\partial_x(t,\alpha)}{\partial(t,\alpha)}$, $\quad \alpha = q$. Then by using (2.25) we have

$$\begin{aligned} \frac{\partial}{\partial t} \ln \Big(\det \frac{\partial_x(t,\alpha)}{\partial(t,\alpha)}\Big) &= \mathrm{tr}\bigg(\Big(\frac{\partial_x(t,\alpha)}{\partial(t,\alpha)}\Big)^{-1} \frac{\partial}{\partial t}\Big(\frac{\partial_x(t,\alpha)}{\partial(t,\alpha)}\Big)\bigg) \implies \\ \frac{\partial}{\partial t} \ln \mathrm{J}(t,\alpha) &= \mathrm{tr}\bigg[\Big(\frac{\partial_x(t,\alpha)}{\partial(t,\alpha)}\Big)^{-1} \nabla_x f\big(x(t,\alpha)\big)\Big(\frac{\partial_x(t,\alpha)}{\partial(t,\alpha)}\Big)\bigg] = \\ \mathrm{tr}\bigg[\Big(\frac{\partial_x(t,\alpha)}{\partial(t,\alpha)}\Big)^{-1}\Big(\frac{\partial_x(t,\alpha)}{\partial(t,\alpha)}\Big)\nabla_x f\big(x(t,\alpha)\big)\bigg] &= \mathrm{tr}\Big(\nabla_x f\big(x(t,\alpha)\big)\Big) = \nabla \cdot f\big(x(t,\alpha)\big) \ , \end{aligned} \tag{A.6}$$

since $\mathrm{tr}(BC) = \mathrm{tr}(CB)$.

- Now we consider the Hamiltonian system for the rays

$$\begin{cases} \frac{d\bar{x}}{dt} = \bar{k}(t,\alpha) \ , \\ \\ \frac{d\bar{k}(t,\alpha}{dt} = -\mathrm{V}'\big(\bar{x}(t,\alpha)\big) \ . \end{cases}$$

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