Quantum Hydrodynamics of Gaussian Wavepackets

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Abstract

We study some basic aspects of the quantum hydrodynamics of Gaussian wave packets which evolve according to the linear Schrödinger equation. In particular we calculate Bohms' quantum potential and the deviation between classical and quantum trajectories for the free particle, for a particle moving in linear potential and a particle trapped by a quadratic potential (harmonic oscillator). In the first two cases all calculations are performed analytically, but in the third case the deviation is computed numerically. The calculations imply some qualitative relation between the spectrum of the Schrödinger equation and the behaviour of the deviation, which must be further investigated for more complicated potentials like, for example, the quartic oscillator.

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

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Περίληψη

Μελετάμε κάποια βασικά στοιχεία κβαντικής υδρομηχανικής κυματοπακέτων Gauss που εξελίσονται σύμφωνα με την γραμμική εξίσωση Schrödinger. Πιο συγκεκριμένα, υπολογίζουμε το κβαντικό δυναμικό Bohm και την απόκλιση μεταξύ κλασσικών και κβαντικών τροχιών για το ελεύθερο σωματίδιο, σωματίδιο που κινείται σε γραμμικό δυναμικό και σωματίδιο παγιδευμένο από τετραγωνικό δυναμικό (αρμονικός ταλαντωτής). Στις πρώτες δύο περιπτώσεις όλοι οι υπολογισμοί έχουν γίνει αναλυτικά, όμως στην τρίτη περίπτωση η απόκλιση έχει υπολογιστεί αριθμητικά. Οι υπολογισμοί αυτοί υπονοούν ποιοτικό συσχετισμό ανάμεσα στο φάσμα της εξίσωσης Schrödinger και την συμπεριφορά της απόκλισης των τροχιών, το οποίο πρέπει να διερευνηθεί περαιτέρω για πιο πολύπλοκα δυναμικά, παραδείγματος χάριν τετάρτης τάξης (αναρμονικός ταλαντωτής).

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

Contents

List of Figures

Part I

Quantum mechanics & quantum hydrodynamics

CHAPTER 1

Introduction

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

$$i\varepsilon\partial_t\psi^\varepsilon(x,t) = \left(-\frac{\varepsilon^2}{2}\partial_x^2 + V(x)\right)\psi^\varepsilon(x,t), \quad x\in\mathbb{R}\,,\ t>0\,, \quad \psi^\varepsilon(x,0)=\psi_0^\varepsilon(x) \tag{1.1}$$

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, the "position-space wave function"). The operator $\left(-\frac{\varepsilon^2}{2}\partial_x^2 + V(x)\right)$ is the quantization of the standard Hamiltonian function $H(x,k)=\frac{k^2}{2}+V(x)$, that is the total energy, which equals kinetic energy plus potential energy, of the corresponding classical particle. The parameter ε does not necessarily coincide with the Planck's constant, but it is a small parameter encoding also the space-time scales of the physical problem and the typical wave length of oscillations of the initial data. This problem is of fundamental importance in quantum mechanics [Gr], and classical wave propagation, for example, in long range paraxial wave propagation in inhomogeneous media [Tap].

The initial data of interest usually are oscillatory or oscillatory-localized, namely, either of WKB type [BLP]

$$\psi_0^\varepsilon(x) = A_0(x)e^{\frac{i}{\varepsilon}\Phi_0(x)}\,, \quad A_0\,,\Phi_0 \text{ real functions} \tag{1.2}$$

or of Gaussian form

$$\psi_0^\varepsilon(x) = \mathrm{N}\exp\left(-\alpha_0(x-x_0)^2+\frac{i}{\varepsilon}p_0(x-x_0)\right)\,,\ \alpha_0>0\,,\ p_0\in\mathbb{R}\,. \tag{1.3}$$

We are interested in the high-frequency solution of (1.1), that is the expansion of ψ^ε in the regime $\varepsilon\ll 1$, which is referred to as the the *semi-classical limit*. The limit case where we consider that $\varepsilon\to 0$ will be referred to as the the *classical limit* (or the *geometrical-optics solution*). The mode of transition from the semiclassical regime to the classical limit 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, and it also depends crucially on the structure of the initial data.

1.1 WKB method, geometrical optics and caustics

In the case of WKB initial data (1.2), an approximation is constructed by the WKB method (or "geometrical optics" method) which is based on the ansatz

$$\psi^\varepsilon(\mathbf{x},t) \approx A(x,t)e^{\frac{i}{\varepsilon}\Phi(x,t)} \,. \tag{1.4}$$

It turns out that the phase satisfies the Hamilton-Jacobi equation (see Appendix A)

$$\partial_t\Phi + \frac{1}{2}\big(\partial_x\Phi\big)^2 + V = 0 \,, \tag{1.5}$$

and the amplitude satisfies the transport equation

$$\partial_t A^2 + \partial_x\big(A^2\partial_x\Phi\big) = 0 \,, \tag{1.6}$$

with initial data $A(x,0) = A_0(x)$, $\Phi(x,0) = \Phi_0(x)$, respectively.

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 the amplitude $A(x,t)$ becomes infinite, or in shadow regions (i.e. regions devoid of rays) where it yields zero fields, and the phase function $\Phi(x,t)$ becomes, in general, multivalued. 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. Assuming that the multivalued phase function is known, uniform asymptotic formulas for the wave field near the caustics have been constructed using boundary layer techniques [BAKI], [BB] as well as phase space techniques, and notably Lagrangian integrals [Lu], [Kra], [DUI], [GS], [KO], and the method of canonical operator [MF]. A relatively new phase-space technique for studying oscillatory solutions of dispersive wave equations and the homogenization of energy density $\eta^\varepsilon(x,t) =\mid \psi^\varepsilon(x,t) \mid^2$, is based on the use of the Wigner transform (see, e.g., [GM], [GMMP]). A construction of the Wigner function and a detailed study of its behaviour near simple caustics has been presented in [FM].

1.2 Wavepackets and Gaussian beams

A different asymptotic method, which, in principle, allows to avoid caustic singularities is the Gaussian beam method which is based on the propagation of certain Gaussian wave packets along the bicharacteristics of the Hamiltonian system associated with the solution of the Hamilton-Jacobi equation. The Gaussian wave packets are approximate solutions to the Schrödinger equation with suitably defined harmonic potentials and initial data (1.3). The most important feature of the method is that the phase of the asymptotic ansatz is complex, thus providing the flexibility to avoid the caustics living in real physical space-time. Efficient solutions of the semiclassical Schrödinger equation have been constructed either by summation of Gaussian beams, a method or by the wavepacket transform. Both methods start from the decomposition of general initial data into the (discrete or integral) sum of Gaussian wave packets (see, e.g., [BB], [Ral],[KKL], [NSS])

1.3 Quantum hydrodynamics, de Broglie-Bohm theory and pilot waves

An astonishing analogy between a time-dependent quantum particles and a "quantum" fluid system which is pseudo-barotropic, irrotational and inviscid, was established by Madelung [Mad] in 1927, a year after Erwin Schrödinger published his celebrated equation. He found that the velocity potential satisfies the Hamilton-Jacobi type equation (1.5) with an additional term, the quantum potential, and he interpreted this potential

as an "internal" force of the "quantum" fluid. In fact, a pressure-like term can be extracted from the Bohm potential, and it has been shown that the existence of a pressure gradient force in the fluid description does not violate Ehrenfest's theorem since its expectation value is zero. The Madelung equations describe a compressible fluid, and compressibility yields a linkage between hydrodynamic and thermodynamic effects. The work done by the pressure gradient force to expand the flow transforms internal thermal microscopic kinetic energy to the macroscopic hydrodynamic kinetic energy of the flow. Such thermodynamic aspects of Madelung's theory in relation to emergent quantum mechanics have been the subject of intensive research in recent years. See, e.g., [Gros1], [Gros2] [HC].

In 1952, Bohm [Boh] in the framework of his pioneering investigations of de Broglie's pilot wave theory [Bro], rediscovered Madelung's equations. According to pilot wave theory quantum particles are borne along on some type of wave. The de Broglie–Bohm theory describes particles moving under the guidance of Schrödinger 's wave function. In de Broglie's original formulation, the particle dynamics is given by a first-order differential equation. In Bohm's reformulation, it is given by Newton's law of motion with an extra potential that depends on the quantum potential—together with a constraint on the possible velocities. Thus quantum hydrodynamic equations provided the mathematical framework for pilot wave theory. According to pilot-wave theory, the particles have definite trajectories, but because of the pilot wave's influence, they still exhibit wavelike statistics. In the past decade, Bush [Bu1], [Bu2], [Bu3] has considered the pilot-wave theory in relation to the first hydrodynamic analogs of single-particle quantum systems that have emerged from exciting experiments by Couder et al [CPFB] that show quantum-like behaviour of liquid droplets bouncing and walking on the free surface of a fluid.

On the mathematical side, Bohmian mechanics, an alternative term for quantum hydrodynamics, and especially its relation to classical mechanics- the so called classical limit- has been investigated by Markowich and his collaborators [MPS1], [MPS2], [FKMS]. These authors invented novel functional-analytic tools, namely the Bohmian measures, to characterise the weak convergence of quantum particle trajectories to their classical counterparts. In a related direction, Dürr & Römer [DR] have shown convergence in probability when Schrödinger 's wave function is approximated by a Gaussian wavepacket.

1.4 Scope of the thesis

In this work we aim to get, through explicit computations in simple cases, some insight into the quantum potential and the Bohmian trajectories, assuming that the evolution of the Schrödinger wavefunction is reasonably approximated by a Gaussian wavepacket. In this respect the title of this work could have been *"Remarks on the quantum hydrodynamics of Gaussian wavepackets"*.

In particular, we consider three different cases for the potential V, namely, the zero, the linear and the quadratic potential, and we compute the deviation between the Bohmian and the classical trajectories. This deviation is governed by a second order ordinary differential equation with time-dependent coefficients. In all cases we are able to compute the quantum potential in explicit form. However, the deviation of trajectories is computed explicitly only for the zero and linear potential, and it is found that it increases with time. In the case of quadratic potential the coefficient of the governing ODE is periodic, and the deviation is computed numerically. In this case we are not able to check analytically if the deviation remains bounded for all times, because we lack necessary conditions for the boundedness of the solution of the corresponding ODE. Nevertheless, numerical computations imply bounded oscillatory deviation between Bohmian and classical trajectories. We conjecture that the observed qualitative behaviour stems from the fact that the spectrum of the Schrödinger equation for the quadratic potential is discrete, while in the other two cases is continuous.

The structure of the work is as follows. In Chapter 2 we present briefly the wave packet approximation of the evolving wave function. In Chapter 3 we derive the equations of quantum hydrodynamics and Bohmian trajectories. In Chapter 4 we present with details the computations of the quantum potential and the deviation between classical and Bohmian trajectories for the aforementioned potentials. In the last Chapter 5 we

attempt a discussion of the results and a description of open questions that should be addressed for the understanding the quantum hydrodynamics of Gaussian beams evolving in more general potentials, as well as the hydrodynamics of other beam-like solutions of the Schrödinger equation.

CHAPTER 2

Quantum Hydrodynamics

2.1 Bohm equations and quantum potential

Following Madelung [Mad] we decompose the Schrödinger equation into two real equations, by writing the complex-valued time-dependent wave function in the polar form

$$\psi^\varepsilon(x,t) = \mathrm{R}^\varepsilon(x,t)e^{\frac{i}{\varepsilon}\mathrm{S}^\varepsilon(x,t)} \,, \tag{2.1}$$

where

$$\mathrm{R}^\varepsilon(x,t) = |\psi^\varepsilon(x,t)| \,, \tag{2.2}$$

is the amplitude, and

$$\mathrm{S}^\varepsilon(x,t) = \varepsilon \arg \psi^\varepsilon(x,t) = \varepsilon \mathrm{Im}(\ln \psi^\varepsilon(\mathrm{x},\mathrm{t})) \,, \tag{2.3}$$

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

Substituting (2.1) into the Schrödinger equation (1.1) we obtain

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

and separating the last equation into its real and imaginary parts we get the following equations

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

and

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

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

$$\partial_t \mathrm{S}^\varepsilon + \frac{1}{2}\big(\partial_x \mathrm{S}^\varepsilon\big)^2 + V + Q^\varepsilon = 0 \,, \tag{2.4}$$

$$\partial_t\big(\mathrm{R}^\varepsilon\big)^2 + \partial_x \cdot \Big(\big(\mathrm{R}^\varepsilon\big)^2 \partial_x \mathrm{S}^\varepsilon\Big) = 0 \,, \tag{2.5}$$

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

$$Q^\varepsilon = -\frac{\varepsilon^2}{2}\frac{\partial_x^2 \mathrm{R}^\varepsilon}{\mathrm{R}^\varepsilon} \,. \tag{2.6}$$

The system (2.4), (2.5) 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 the way of their derivation, these equations are equivalent to the Schrödinger equation. As such, they have been used as the basis for various alternative approaches in quantum mechanics, as hidden variable theory [Boh] and de Broglie's pilot wave theory [Hol], [DT], but also for computational purposes, e.g. in quantum chemistry [Wy].

In addition to the comments and the remarks we made in Section 1.3 concerning the physical foundations of the quantum potential, it is interesting to observe, that from its definition (2.6), it follows that the amplitude R^ε satisfies the equation

$$\frac{\varepsilon^2}{2}\frac{\partial^2 \mathrm{R}^\varepsilon}{\partial x^2} + Q^\varepsilon(x,t)\mathrm{R}^\varepsilon = 0 \,. \tag{2.7}$$

The character of this non-linear equation may change from elliptic to hyperbolic since, in general, the quantum potential changes sign, and, at least qualitatively, the behaviour of this equation can be related to the properties of the geometrical optics' rays and the behaviour of the WKB solution. See, e.g., [Car1], [Car2], [Car3] for certain mathematical aspects of this equation and their relations to the role of quantum potential in emergent quantum mechanics.

Since the quantum potential is expressed through the amplitude R^ε, it turns out that it admits different approximations for various approximations of the wave function. It is instructive to observe that for the WKB solution (1.4) the quantum potential is

$$Q^\varepsilon(x,t) = -\frac{\varepsilon^2}{2}\frac{\partial_x^2 A}{A} \,, \tag{2.8}$$

where A, the solution of the transport equation (1.6), is independent of the semiclassical parameter ε. Therefore, whenever A is bounded, Q^ε, at least formally, disappears as $\varepsilon \to 0$. But, in general, this is not true when there are caustics where A becomes infinite (see Appendix A). In this situation there is a boundary layer near the caustic, where (2.8) does not converge to zero, and A, Φ are not correct solutions to Bohm equations [Karn].

Concerning the correct choice of the initial data for the Bohm equations, from the WKB initial data for (1.2) we obtain the initial data

$$\mathrm{R}^\varepsilon(x,0) = A_0(x) \,, \qquad \mathrm{S}^\varepsilon(x,0) = \Phi_0(x) \,, \tag{2.9}$$

while from the Gaussian data (1.3) we obtain the initial data

$$\mathrm{R}^\varepsilon(x,0) = -\alpha_0(x-x_0)^2 \,, \qquad \mathrm{S}^\varepsilon(x,0) = p_0(x-x_0) \,, \tag{2.10}$$

which are independent of ε. Although the initial data are independent of ε, the solutions of Bohm equations do depend on ε because of the quantum potential. Of course, ε- dependent initial data may also be devised either for certain physical applications or technical mathematical reasons.

2.2 Hydrodynamic variables and the role of quantum potential

We recall now the Euler equations

$$\partial_t \rho + \partial_x(\rho u) = 0 \quad \text{(conservation of mass)} , \tag{2.11}$$

$$\rho(\partial_t u + u\partial_x u) = -\partial_x \Pi + \rho b \quad \text{(conservation of momentum)} , \tag{2.12}$$

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

We consider now a fluid with density

$$\rho^\varepsilon = (\mathrm{R}^\varepsilon)^2 , \tag{2.13}$$

and Eulerian velocity

$$z^\varepsilon = \partial_x \mathrm{S}^\varepsilon . \tag{2.14}$$

For brevity, we refer to this fluid as the *quantum fluid*, but one should be very careful to avoid confusion with real fluids where quantum effects are important for the flow. Then, the transport equation (2.5) is written in the form

$$\partial_t \rho^\varepsilon + \partial_x(\rho^\varepsilon z^\varepsilon) = 0 . \tag{2.15}$$

By the identification

$$\rho = \rho^\varepsilon , \;\; u = z^\varepsilon , \tag{2.16}$$

we see that equation (2.15) coincides with the continuity equation (2.11).

Furthermore, by differentiating (2.4) with respect to x, and using the definition (2.14) of the fluid velocity, we derive the following inhomogeneous Burgers equation for the velocity

$$\frac{dz^\varepsilon}{dt} = \partial_t z^\varepsilon + z^\varepsilon \partial_x z^\varepsilon = -\partial_x(Q^\varepsilon + V) , \;\; z^\varepsilon := \partial_x S^\varepsilon . \tag{2.17}$$

We again use the identification (2.16) and we compare (2.17) with (2.12). It turns out that the pressure p^ε of the quantum fluid must satisfy

$$\partial_x \Pi^\varepsilon = \rho^\varepsilon \partial_x Q^\varepsilon , \tag{2.18}$$

and $b^\varepsilon = -\frac{\partial_x V}{\eta^\varepsilon}$. We rewrite the quantum potential (2.6) in the form

$$Q^\varepsilon = -\frac{\varepsilon^2}{4}\left(\frac{1}{2}(\partial_x \ln \rho^\varepsilon)^2 + \partial_x^2 \ln \rho^\varepsilon\right) , \tag{2.19}$$

in terms of the density. We differentiate the last equation with respect to x, and compare the resulting equation with (2.18). It follows that the quantum pressure depends only on the density

$$\Pi^\varepsilon = -\frac{\varepsilon^2}{4}\rho^\varepsilon \partial_x^2 \ln \rho^\varepsilon , \tag{2.20}$$

that is the "quantum" fluid is pseudo-barotropic, because the pressure is not a function of the density only, but it also depends on the derivatives of the pressure.

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)[Boh]. See also [DT] for a detailed mathematical approach to Bohmian mechanics and quantum potentials, and [Wy] for an exposition of quantum hydrodynamics from the point of view of quantum chemistry.

2.3 Bohm trajectories

The *Bohmian trajectories* are defined as the characteristics of the equation

$$\frac{dz^\varepsilon}{dt} = \partial_t z^\varepsilon + z^\varepsilon \partial_x z^\varepsilon = -\partial_x (V + Q^\varepsilon) \,, \quad z^\varepsilon = \partial_x S^\varepsilon. \tag{2.21}$$

They satisfy the system

$$\begin{cases} \frac{dx^\varepsilon(t;q,p)}{dt} = p^\varepsilon(t;q,p) \,, \\ \\ \frac{dp^\varepsilon(t;q,p)}{dt} = -\partial_x (V + Q^\varepsilon)\big(x^\varepsilon(t;q,p),t\big) \,, \\ \\ x^\varepsilon(0;q) = q, \qquad p^\varepsilon(0;q) = z^\varepsilon(q,0) = (S^\varepsilon(q,0))' \,. \end{cases} \tag{2.22}$$

In de Broglie-Bohm theory the quantum particle moves along these trajectories driven by the pilot wave which is described by the Schrödinger wave function.

When the ray field is smooth and there are no caustics, it has been shown that the Bohm trajectories exist globally in time ([TT], [BDGPZ], [Be]), they converge to the rays as $\varepsilon \to 0$, and the solution of the Burgers equation (2.21) converges to the derivative of the solution of the Hamilton-Jacobi equation (1.5) ([FKMS], [MPS1], [MPS2]; see also [Boh] for the physical content of the convergence). However, such convergence results cannot be proved after caustic formation, and as it has been shown by specific examples that even the Bohmian trajectories may be not well defined [Karn].

CHAPTER 3

Wave-packet approximation of the wavefunction

In this chapter we briefly present the Gaussian wave packet approximation of the Schrödinger wavefunction. We restrict ourselves in the one dimensional case, and we closely follow the exposition by Tannor [Tan].

3.1 Construction of the wavepacket

We assume that the initial wave packet

$$\psi^\varepsilon(x,0) = \psi_0^\varepsilon(x) = \mathrm{N}\exp\Big(-\alpha_0(x-x_0)^2 + \frac{i}{\varepsilon}p_0(x-x_0)\Big)\,, \tag{3.1}$$

which is localized at the phase-space point (x_0, p_0), evolves to the Gaussian wave packet

$$\psi^\varepsilon(x,t) = \mathrm{N}\exp\Big(-\alpha_t(x-x_t)^2 + \frac{i}{\varepsilon}p_t(x-x_t) + \frac{i}{\varepsilon}\gamma_t\Big)\,, \tag{3.2}$$

which is localized near the phase-space point (x_t, p_t). The functions $\alpha_t, x_t, p_t, \gamma_t$ will be defined so that $\psi^\varepsilon(x,t)$ satisfies the Schrödinger equation in a certain approximation.

We calculate $\partial_x^2\psi^\varepsilon$ and $\partial_t\psi^\varepsilon$, and we substitute them into the Schrödinger equation. We have that

$$\partial_x^2\psi^\varepsilon = (4\alpha_t^2(x-x_t)^2 - 4\frac{i}{\varepsilon}\alpha_t p_t(x-x_t) - \frac{1}{\varepsilon^2}p_t^2 - 2\alpha_t)\psi^\varepsilon\,, \tag{3.3}$$

and

$$\partial_t\psi^\varepsilon = \psi^\varepsilon(-\dot\alpha_t(x-x_t)^2 + 2\alpha_t\dot x_t(x-x_t) + \frac{i}{\varepsilon}(\dot p_t(x-x_t) - p_t\dot x_t + \dot\gamma_t))\,. \tag{3.4}$$

Moreover, we approximate $V(x)$ near x_t by Taylor's formula

$$V(x) = V(x_t) + V'(x_t)(x-x_t) + \frac{1}{2}V''(x-x_t)^2 + O\big((x-x_t)^3\big)\,. \tag{3.5}$$

By substituting (3.3), (3.4) and (3.5) into Schrödinger equation (1.1), and by equating powers of $(x-x_t)$ we get the following equations:

- By equating coefficients of $(x - x_t)^2$:

$$\dot{\alpha}_t = -2i\varepsilon\alpha_t^2 + \frac{i}{2\varepsilon}V''(x_t) \, .$$

For later convenience we put $\alpha_t = -\frac{i}{2\varepsilon}A_t$, and we get the Riccati equation

$$\dot{A}_t + A_t^2 + V''(x_t) = 0 \, , \tag{3.6}$$

which must satisfy the initial data $A_0 = 2\varepsilon\alpha_0 i$.

- By equating coefficients of $(x - x_t)$:

$$2i\varepsilon\alpha_t(\dot{x}_t - p_t) - \dot{p}_t = V'(x_t) \, . \tag{3.7}$$

The last equation is automatically satisfied by choosing x_t, p_t such that

$$\begin{cases} \dot{x}_t = p_t \, , \\ \\ \dot{p}_t = -V'(x_t) \, , \end{cases} \tag{3.8}$$

which is the Hamiltonian system $(A.12)$ defining a classical trajectory $x_t = x(t; x_0, p_0), p_t = k(t; x_0, p_0)$. The initial point of the trajectory must be the base point (x_0, p_0) of the initial wavepacket in order for (3.2) to satisfy at $t = 0$ the initial data (3.1). Therefore, the wave packet moves along the trajectory emanating at the point $(x = x_0, p = p_0)$ of phase space.

Remark. It is important to note that this trajectory coincides with the bicharacteristic of the Hamilton-Jacobi equation (1.5) with initial data $\Phi(x, 0) = p_0(x - x_0)$, see eq (2.10).

- By equating coefficients of $(x - x_t)^0$:

$$\dot{\gamma}_t = \mathcal{L}_{cl} - \varepsilon^2\alpha_t = \mathcal{L}_{cl} + \frac{i\varepsilon}{2}A_t \, , \tag{3.9}$$

where $\mathcal{L}_{cl} = \frac{1}{2}\dot{x}_t^2 - V(x_t)$ is the classical Lagrangian of the system.

By integrating (3.9) we get

$$\gamma_t = S(t) + \frac{i\varepsilon}{2}\int_0^t A_t dt \, , \tag{3.10}$$

where

$$S(t) = \int_0^t \left(\frac{1}{2}\dot{x}_t^2 - V(x_t)\right) dt \, ,$$

is the classical action integral along the trajectory x_t. Note that the action S is the solution $(A.19)$ of the Hamilton-Jacobi equation $(A.17)$.

Finally, it is convenient to rescale α_0 to $\frac{\alpha_0}{2\varepsilon}$ which implies $A_0 = i\alpha_0$. Then ψ^ε and ψ_0^ε assume the form

$$\psi^\varepsilon(x, t) = \mathrm{N}\exp\left(\frac{i}{2\varepsilon}A_t(x - x_t)^2 + \frac{i}{\varepsilon}p_t(x - x_t) + \frac{i}{\varepsilon}\gamma_t\right) \, , \tag{3.11}$$

and

$$\psi^\varepsilon(x, 0) = \psi_0^\varepsilon(x) = \mathrm{N}\exp\left(\frac{i}{2\varepsilon}A_0(x - x_0)^2 + \frac{i}{\varepsilon}p_0(x - x_0)\right) \, , \tag{3.12}$$

respectively.

3.2 The solution of Riccati equation

In order to solve the Riccati equation (3.6),

$$\dot{A}_t + A_t^2 + V''(x_t) = 0 \,, \quad A_0 = i\alpha_0 \,,$$

we use the representation $A_t = \frac{b}{c}$ where the functions b and c will be chosen in an appropriate way. We substitute this ansatz in (3.6) and we get the equation

$$\dot{b}c - b\dot{c} + b^2 + V''c^2 = 0 \,.$$

The last equation is automatically satisfied by choosing b, c so that

$$\begin{cases} \dot{b} = -V''c \,, \\ \\ \dot{c} = b \,. \end{cases} \tag{3.13}$$

Thus, we derive the solution of the Riccati equation by solving the system

$$\begin{cases} \ddot{c} + V''c = 0, \ c(0) = 1 \,, \\ \\ \dot{c} = b, \ b(0) = \dot{c}(0) = i\alpha_0 \,. \end{cases} \tag{3.14}$$

Note that this system is the variational (stability) system corresponding to the Hamiltonian system $(A.12)$[1].

[1] In general the variational equations are coupled. In the simple case we study, they are uncoupled since we consider the standard separable Hamiltonian.

Part II

Bohmian mechanics in the wave packet approximation

CHAPTER 4

Quantum potential and Bohmian trajectories

In this chapter we compute the quantum potential and the corresponding Bohmian trajectories for simple external potentials V, assuming that the wave function is approximated by the Gaussian wave packet described in previous chapters. More precisely, in order to gain some physical insight into the trajectories we compute the deviation between the Bohmian trajectories and the classical trajectories, the later being the rays of geometrical optics.It may be considered that this deviation describes the influence of quantum effects to the energy propagation, and, in a sense, is not necessarily ignorable for small ε.

The amplitude of the wave function (3.11) is

$$\begin{aligned} \mathrm{R}^\varepsilon(x,t) = |\psi^\varepsilon| &= \mathrm{N}\exp\left(\mathrm{Re}\left(\frac{i}{2\varepsilon}A_t(x-x_t)^2 + \frac{i}{\varepsilon}p_t(x-x_t) + \frac{i}{\varepsilon}\gamma_t\right)\right) \\ &= \mathrm{N}\exp\left(-\frac{1}{2\varepsilon}(\mathrm{Im}A_t)(x-x_t)^2 - \frac{1}{\varepsilon}\mathrm{Im}\gamma_t\right) , \end{aligned}$$

which, by using (3.10), is written in the form

$$\mathrm{R}^\varepsilon = \mathrm{N}\exp\left(-\frac{1}{2\varepsilon}(\mathrm{Im}A_t)(x-x_t)^2 - \frac{1}{2}\int_0^t \mathrm{Re}A_t dt\right) . \tag{4.1}$$

The phase of the wavefunction is given by (3.11) and (2.3),

$$\mathrm{S}^\varepsilon(x,t) = \frac{1}{2}(\mathrm{Re}A_t)(x-x_t)^2 + p_t(x-x_t) + \frac{d}{dt}(\mathrm{Re}\gamma_t) , \tag{4.2}$$

and therefore the Eulerian velocity z^ε is

$$\mathrm{z}^\varepsilon(x,t) = \partial_x \mathrm{S}^\varepsilon(x,t) = (\mathrm{Re}A_t)(x-x_t) + p_t . \tag{4.3}$$

As it is expected the velocity z^ε is equal to the classical velocity p_t along the classical trajectory. It is important to note that for $t=0$, we have $\mathrm{Re}A_0 = 0$, and therefore by (2.22), for any q, we have

$$p_0^\varepsilon(0;q) = \mathrm{z}^\varepsilon(q,0) = p_0 . \tag{4.4}$$

In order to calculate Q^ε given by (2.6), we need to calculate $\partial_x^2 \mathrm{R}^\varepsilon$. We have that

$$\partial_x \mathrm{R}^\varepsilon = \mathrm{R}^\varepsilon \partial_x \left(-\frac{1}{2\varepsilon}(\mathrm{Im}A_t)(x-x_t)^2 - \frac{1}{2}\int_0^t \mathrm{Re}A_t dt\right)$$

$$= \mathrm{R}^\varepsilon \left(-\frac{1}{\varepsilon}(\mathrm{Im}A_t)(x - x_t) \right) , \tag{4.5}$$

and

$$\begin{aligned} \partial_x^2 \mathrm{R}^\varepsilon &= \partial_x \mathrm{R}^\varepsilon \left(-\frac{1}{\varepsilon}(\mathrm{Im}A_t)(x - x_t) \right) + \mathrm{R}^\varepsilon \partial_x \left(-\frac{1}{\varepsilon}(\mathrm{Im}A_t)(x - x_t) \right) \\ &= \mathrm{R}^\varepsilon \left(\left(-\frac{1}{\varepsilon}(\mathrm{Im}A_t)(x - x_t) \right)^2 - \frac{1}{\varepsilon}\mathrm{Im}A_t \right) \\ &= \mathrm{R}^\varepsilon \left(\left(\frac{1}{\varepsilon^2}(\mathrm{Im}A_t)^2(x - x_t)^2 \right) - \frac{1}{\varepsilon}\mathrm{Im}A_t \right) . \end{aligned} \tag{4.6}$$

Thus we obtain

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

By defining

$$\omega_t = \mathrm{Im}A_t , \tag{4.7}$$

we get

$$Q^\varepsilon = -\frac{1}{2}\omega_t^2(x - x_t)^2 + \frac{1}{2}\varepsilon\omega_t . \tag{4.8}$$

It turns out that, in the wave packet approximation of the wave function, the quantum potential is harmonic with *time dependent frequency* ω_t. The frequency is expressed through the solution of the Riccati equation (3.6), and the bottom of the quantum potential is moving along the classical trajectory.

Substituting (4.8) into (2.22), we get the following system for the Bohmian trajectories

$$\begin{cases} \dot{x}_t^\varepsilon = p_t^\varepsilon , \\ \\ \dot{p}_t^\varepsilon = -V'(x_t^\varepsilon) + \omega_t^2(x_t^\varepsilon - x_t) . \end{cases} \tag{4.9}$$

Combining the classical Hamiltonian system (3.8) with (4.9) we get

$$\begin{cases} \dot{x}_t^\varepsilon - \dot{x}_t = p_t^\varepsilon - p_t , \\ \\ \dot{p}_t^\varepsilon - \dot{p}_t = -\left(V'(x_t^\varepsilon) - V'(x_t)\right) + \omega_t^2(x - x_t) . \end{cases} \tag{4.10}$$

Now by using Taylor's formula we have

$$V'(x_t^\varepsilon) - V'(x_t) = V''(x_t)(x_t^\varepsilon - x_t) + O\left((x_t^\varepsilon - x_t)^2\right) ,$$

and we approximate the second equation of (4.10) by

$$\dot{p}_t^\varepsilon - \dot{p}_t = \left(\omega_t^2 - V''(x_t)\right)(x_t^\varepsilon - x_t) . \tag{4.11}$$

We now introduce the new variables

$$y_t^\varepsilon = x_t^\varepsilon - x_t , \quad \xi_t^\varepsilon = p_t^\varepsilon - p_t , \tag{4.12}$$

representing the *deviation between classical and Bohmian trajectories*. Obviously they satisfy the linear system

$$\begin{cases} \dot{y}_t^\varepsilon = \xi_t^\varepsilon \ , \\ \\ \dot{\xi}_t^\varepsilon = \left(\omega_t^2 - V''(x_t)\right) y_t^\varepsilon \ . \end{cases} \tag{4.13}$$

Assuming that $x_t^\varepsilon = x_0^\varepsilon$ for $t = 0$, by (4.4) and the remark after (3.8), the initial data of the deviation must be specified as

$$y_0^\varepsilon = x_0^\varepsilon - x_0 \ , \quad \xi_0^\varepsilon = p_0^\varepsilon - p_0 = 0 \ . \tag{4.14}$$

Thus, y_t^ε is found form the solution of the linear initial value problem

$$\ddot{y}_t^\varepsilon = \left(\omega_t^2 - V''(x_t)\right) y_t^\varepsilon \ , \ \ y_0^\varepsilon = x_0^\varepsilon - x_0 \ , \ \ \dot{y}_0^\varepsilon = 0 \ . \tag{4.15}$$

Therefore, for the computation of the deviation between the trajectories, we need to compute only the classical trajectories and the solution of the Ricatti equation. It also turns out that, in general, the Bohmian trajectory starting at x_0, i.e. $y_0^\varepsilon = 0$, coincides with the classical trajectory starting at the same point, assuming enough regularity of the coefficient $\left(\omega_t^2 - V''(x_t)\right)$.

In the sequel we compute the quantum potential Q^ε, the Eulerian velocity z^ε and, most informative, the deviation y_t^ε, in three basic cases, namely for a free particle, a particle moving in linear external potential and the harmonic oscillator.

4.1 Example 1: The free particle

In this case, $V \equiv 0$, all the computations can be performed analytically, and we recover the results already derived by Pan[Pan].

The solution of the Hamiltonian system

$$\begin{cases} \dot{x}_t = p_t, \ \ x_t(0) = x_0 \ , \\ \\ \dot{p}_t = 0, \ \ p_t(0) = p_0 \ , \end{cases} \tag{4.16}$$

is elementary, and it is given by

$$\begin{cases} x_t = p_0 t + x_0 \ , \\ \\ p_t = p_0 \ . \end{cases} \tag{4.17}$$

The solution of the Riccati equation is also elementary since $V'' \equiv 0$, and the system for b, c simplifies to

$$\begin{cases} \ddot{c} = 0, \ c(0) = 1 \ , \\ \\ \dot{c} = b, \ b(0) = \dot{c}(0) = i\alpha_0 \ . \end{cases} \tag{4.18}$$

The solution of the previous system is given by

$$\begin{cases} c(t) = i\alpha_0 t + 1 \ , \\ \\ b(t) = i\alpha_0 \ , \end{cases} \tag{4.19}$$

and the solution of the Riccati equation is

$$A(t) = \frac{b(t)}{c(t)} = \frac{i\alpha_0}{i\alpha_0 t + 1} = \frac{\alpha_0^2}{1 + \alpha_0^2 t^2} + \frac{i\alpha_0}{1 + \alpha_0^2 t^2} \ . \tag{4.20}$$

Then by (3.1) we have

$$S(t) = \int_0^t \left(\frac{1}{2}\dot{x}_t^2 - V(x_t)\right) dt = \int_0^t \frac{1}{2}p_0^2 dt = \frac{1}{2}p_0^2 t \, .$$

Also

$$\int_0^t A_t dt = \int_0^t \frac{\dot{c}(t)}{c(t)} dt = \ln(c(t)) \, ,$$

and by (3.10)

$$\gamma_t = S(t) + \frac{i\varepsilon}{2}\int_0^t A_t dt = \frac{1}{2}p_0^2 t + \frac{i\varepsilon}{2}\ln(i\alpha_0 t + 1) \, . \tag{4.21}$$

By (4.7) and (4.20), the frequency is

$$\omega_t = \mathrm{Im} A_t = \frac{\alpha_0}{1+\alpha_0^2 t^2} \, . \tag{4.22}$$

Then, by (4.8) and (4.17) the quantum potential is given by

$$Q^\varepsilon = -\frac{1}{2}\frac{\alpha_0^2}{(1+\alpha_0^2 t^2)^2}(x - p_0 t - x_0)^2 + \frac{\varepsilon}{2}\frac{\alpha_0}{(1+\alpha_0^2 t^2)} \, . \tag{4.23}$$

By (4.3) and using (4.20) and (4.17) the Eulerian velocity is

$$\mathrm{z}^\varepsilon(x,t) = \partial_x \mathrm{S}^\varepsilon(x,t) = \frac{\alpha_0^2 t}{(1+\alpha_0^2 t^2)}(x - p_0 t - x_0) + p_0 \, . \tag{4.24}$$

By the change of variable $\tau = \alpha_0 t$, the ODE in (4.15) is rewritten as follows

$$\ddot{y}_\tau^\varepsilon = \frac{1}{(1+\tau^2)^2} y_\tau^\varepsilon \, . \tag{4.25}$$

The previous equation has the general solution

$$y_\tau^\varepsilon = c_1\sqrt{1+\tau^2} + c_2\sqrt{1+\tau^2}\,\arctan\tau \, .$$

Returning to initial variable t we get

$$y_t^\varepsilon = c_1\sqrt{1+\alpha_0^2 t^2} + c_2\sqrt{1+\alpha_0^2 t^2}\,\arctan(\alpha_0 t) \, , \tag{4.26}$$

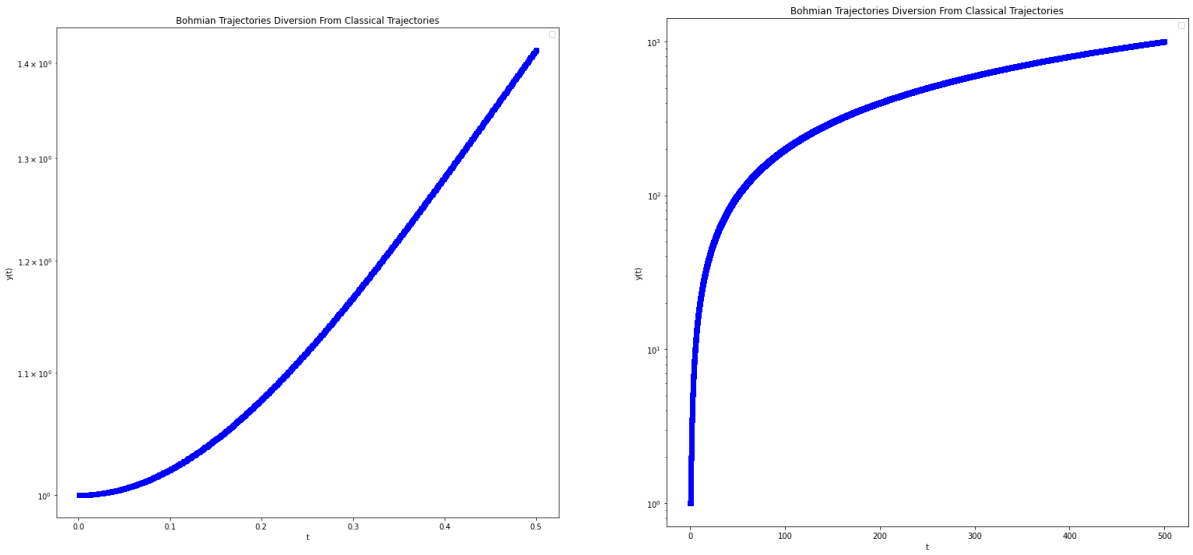
and

$$\dot{y}_\tau^\varepsilon = \frac{y_0^\varepsilon \alpha_0^2 t}{\sqrt{1+\alpha_0^2 t^2}} + c_2\left(\frac{\alpha_0^2 t}{\sqrt{1+\alpha_0^2 t^2}}\arctan(\alpha_0 t) + \frac{1}{\sqrt{1+\alpha_0^2 t^2}}\right) \, . \tag{4.27}$$

By the initial data we obtain $c_1 = y_0^\varepsilon$ and $c_2 = 0$. Thus the solution of (4.15) is

$$y_t^\varepsilon = y_0^\varepsilon\sqrt{1+\alpha_0^2 t^2} \, . \tag{4.28}$$

We observe that the deviation between Bohmian and classical trajectories increase monotonically, and it is almost linear for large time. The typical variation of the deviation is shown in Figure 4, in the case $\alpha_0 = 2$, for small time ($\alpha_0 t < 1$) and for large time ($\alpha_0 t > 1$).



(a) Small time

(b) Large time

Figure. 4.1: *Deviation of trajectories for the free particle*

4.2 Example 2: Linear Potential

In this case, we consider $V = \alpha x$, $\alpha \neq 0$. This problem is of interest, for example,when the quantum particle moves in a constant electric field.

The solution of the Hamiltonian system

$$\begin{cases} \dot{x}_t = p_t, \;\; x_t(0) = x_0 \, , \\ \\ \dot{p}_t = -\alpha, \;\; p_t(0) = p_0 \, , \end{cases} \tag{4.29}$$

is

$$\begin{cases} x_t = -\dfrac{1}{2}\alpha t^2 + p_0 t + x_0 \, , \\ \\ p_t = -\alpha t + p_0 \, . \end{cases} \tag{4.30}$$

Moreover, since again we have $u(t) = V''(x_t) = 0$, as in the case of the free particle, the solution of the Riccati equation is given again by (4.20). This means that the spreading of the Gaussian wave packet, and also the frequency ω_t, are the same in both cases. Therefore it turns out that the deviation between the Bohmian and classical trajectories is the same as for the free particle, although the tractories themselves are quite different.

Also, the geometric phase $S(t)$ and thus γ_t, as well as the quantum potential and the Eulerian velocity, are not the same. This is because they are influenced by the dependence of the classical trajectory on time, which is now quadratic, in contrary to the case of free particle where is linear.

We have

$$\begin{aligned} S(t) &= \int_0^t \left(\frac{1}{2}\dot{x}_t^2 - V(x_t)\right) dt \\ &= \int_0^t \left(\frac{1}{2}(-\alpha t + p_0)^2 - \alpha(-\frac{1}{2}\alpha t^2 + p_0 t + x_0)\right) dt \\ &= \int_0^t \left(\alpha^2 t^2 - 2\alpha p_0 t + \frac{p_0^2}{2} - \alpha x_0\right) dt \\ &= \frac{\alpha^2 t^3}{3} - \alpha p_0 t^2 + \left(\frac{p_0^2}{2} - \alpha x_0\right) t \,, \end{aligned} \tag{4.31}$$

and

$$\gamma_t = \frac{\alpha^2 t^3}{3} - \alpha p_0 t^2 + \left(\frac{p_0^2}{2} - \alpha x_0\right) t + \frac{i\varepsilon}{2}\ln(i\alpha_0 t + 1) \,. \tag{4.32}$$

The quantum potential is

$$Q^\varepsilon = -\frac{1}{2}\frac{\alpha_0^2}{(1+\alpha_0^2 t^2)^2}(x + \frac{1}{2}\alpha t^2 - p_0 t - x_0)^2 + \frac{\varepsilon}{2}\frac{\alpha_0}{(1+\alpha_0^2 t^2)} \,, \tag{4.33}$$

and the Eulerian velocity is

$$\mathrm{z}^\varepsilon(x,t) = \partial_x \mathrm{S}^\varepsilon(x,t) = \frac{\alpha_0^2 t}{(1+\alpha_0^2 t^2)}(x + \frac{1}{2}\alpha t^2 - p_0 t - x_0) - \alpha t + p_0 \,. \tag{4.34}$$

Remark. The quantum potential (4.33) and the velocity (4.24) can be derived independently from the exact wave function constructed for the linear potential in [DaZh] by the versatile operational technique developed in [DaOtToVa]. Therefore the wave packet approximation provides exact solutions in this case.

In the simple case of the free particle, the exact wave function can be constructed in closed form, by using Fourier transform and analytic integration of the Gaussian integral arising in the inversion of the transform.

The aforementioned operational techniques, are essentially selected to handle efficiently the complications associated to the continuous spectrum of the Schrödinger equation when $V \equiv 0$ or $V = \alpha x$.

4.3 Example 3: Quadratic Potential: Harmonic Oscillator

In this case, we consider $V = \frac{1}{2}\omega^2 x^2$, $\omega > 0$. This problem is of interest, for example, when the quantum particle moves in a harmonic trap.

The solution of the Hamiltonian system

$$\begin{cases} \dot{x}_t = p_t, \;\; x_t(0) = x_0 \,, \\ \\ \dot{p}_t = -\omega^2 x_t, \;\; p_t(0) = p_0 \,, \end{cases} \tag{4.35}$$

is

$$\begin{cases} x_t = x_0 \cos(\omega t) + \dfrac{p_0}{\omega}\sin(\omega t) \,, \\ \\ p_t = p_0 \cos(\omega t) - \omega x_0 \sin(\omega t) \,. \end{cases} \tag{4.36}$$

For the harmonic oscillator, in contrary to the cases with zero or linear potential where the trajectories were open, the trajectories are elliptical and periodic.

We have $u(t) = V''(x_t) = \omega^2$, and the functions b, c satisfy the system

$$\begin{cases} \ddot{c} + \omega^2 c = 0,\ c(0) = 1\ , \\ \\ \dot{c} = b,\ b(0) = \dot{c}(0) = i\alpha_0\ . \end{cases} \tag{4.37}$$

The solution of the system is elementary and we get

$$\begin{cases} c(t) = \cos(\omega t) + \dfrac{i\alpha_0}{\omega}\sin(\omega t)\ , \\ \\ b(t) = i\alpha_0\cos(\omega t) - \omega\sin(\omega t)\ . \end{cases} \tag{4.38}$$

Thus, the solution of the Riccati equation is

$$A(t) = \frac{i\alpha_0\cos(\omega t) - \omega\sin(\omega t)}{\cos(\omega t) + \dfrac{i\alpha_0}{\omega}\sin(\omega t)}\ . \tag{4.39}$$

It is also simple to compute the phases

$$S(t) = \int_0^t \left(\frac{1}{2}\dot{x}_t^2 - V(x_t)\right) dt = \frac{p_t x_t - p_0 x_0}{2}\ , \tag{4.40}$$

$$\gamma_t = \frac{p_t x_t - p_0 x_0}{2} + \frac{i\varepsilon}{2}\ln\left(\cos(\omega t) + \frac{i\alpha_0}{\omega}\sin(\omega t)\right)\ . \tag{4.41}$$

Moreover, by writing A_t in the form

$$A_t = \frac{\omega^2\left(\dfrac{\alpha_0^2}{\omega} - \omega\right)\sin(\omega t)\cos(\omega t)}{\omega^2\cos^2(\omega t) + \alpha_0^2\sin^2(\omega t)} + i\frac{\omega^2\alpha_0}{\omega^2\cos^2(\omega t) + \alpha_0^2\sin^2(\omega t)}\ , \tag{4.42}$$

we get the frequency

$$\omega_t = \mathrm{Im}A_t = \frac{\omega^2\alpha_0}{\omega^2\cos^2(\omega t) + \alpha_0^2\sin^2(\omega t)}\ . \tag{4.43}$$

By (4.8) and (4.36) we obtain the quantum potential

$$\begin{aligned} Q^\varepsilon = -\frac{\omega^4\alpha_0^2}{\omega^2\cos^2(\omega t) + \alpha_0^2\sin^2(\omega t)^2}\Big(x - \Big(x_0\cos(\omega t) + \frac{p_0}{\omega}\sin(\omega t)\Big)\Big)^2 \\ + \frac{\omega^2\alpha_0}{\omega^2\cos^2(\omega t) + \alpha_0^2\sin^2(\omega t)}\varepsilon\ . \end{aligned} \tag{4.44}$$

Finally, by (4.3), (4.42) and (4.36) the velocity is given by

$$\begin{aligned} \mathrm{z}^\varepsilon = \partial_x \mathrm{S}^\varepsilon = \frac{\omega^2\left(\dfrac{\alpha_0^2}{\omega} - \omega\right)\sin(\omega t)\cos(\omega t)}{\omega^2\cos^2(\omega t) + \alpha_0^2\sin^2(\omega t)}\Big(x - \big(x_0\cos(\omega t) + \frac{p_0}{\omega}\sin(\omega t)\big)\Big) \\ + p_0\cos(\omega t) - \omega x_0\sin(\omega t)\ . \end{aligned} \tag{4.45}$$

Now, in order to write the equation for the deviation of the trajectories in an appropriate standard form, we use the identities

$$\cos^2(\omega t) = \frac{1+\cos(2\omega t)}{2} ,$$
$$\sin^2(\omega t) = \frac{1-\cos(2\omega t)}{2} ,$$

and we rewrite ω_t in the form

$$\omega_t = \frac{2\omega^2\alpha_0}{(\omega^2+\alpha_0^2)+(\omega^2-\alpha_0^2)\cos(2\omega t)} . \tag{4.46}$$

Thus, the frequency is periodic function with period π/ω. Then, equation (4.15) is given by

$$\ddot{y}_t^\varepsilon = \omega^2 \left(\frac{4\omega^2\alpha_0^2}{\big((\omega^2+\alpha_0^2)+(\omega^2-\alpha_0^2)\cos(2\omega t)\big)^2} - 1 \right) y_t^\varepsilon . \tag{4.47}$$

We rescale the time variable

$$\tau = \omega t ,$$

and we introduce the parameters

$$\sigma = \frac{\omega^2}{\alpha_0^2} , \quad \lambda = \sigma + 1 , \quad \mu = \sigma - 1 .$$

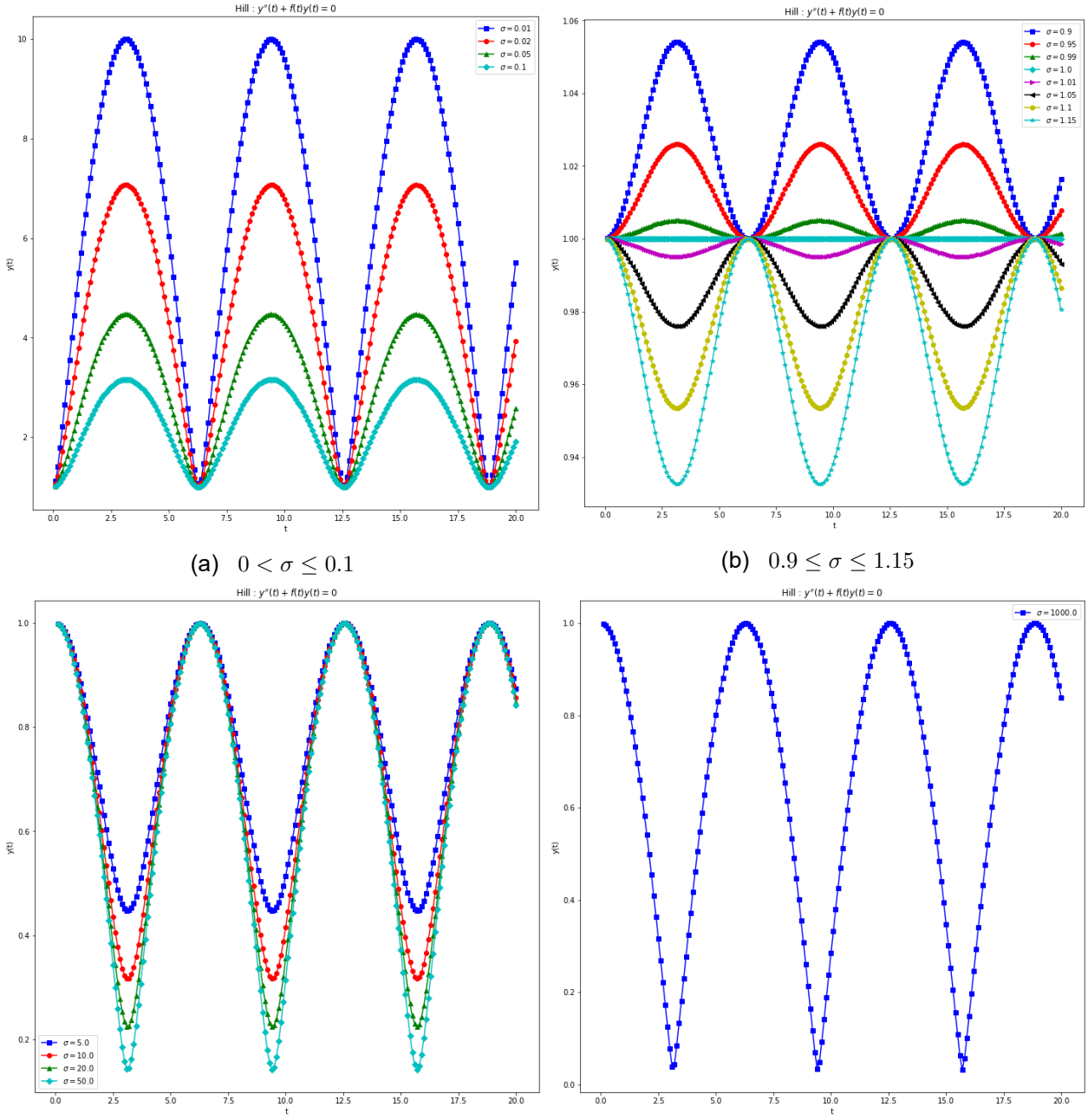
Note that the parameter σ measures the relative scale between the Gaussian width of the initial wave packet and the width of the harmonic well defined by the quadratic potential.

Then, the deviation satisfies the equation

$$\ddot{y}_\tau^\varepsilon = F(\tau) y_\tau^\varepsilon , \quad F(\tau) = \frac{4\sigma}{(\lambda+\mu\cos(2\tau))^2} - 1 . \tag{4.48}$$

This is *Hill's ODE* since $F(\tau+\pi) = F(\tau)$ is periodic. In our case we have also $F(-\tau) = F(\tau)$.

Unfortunately, existing sufficient conditions for the boundedness of the solution do not apply for this particular coefficient F, and we are not aware of any necessary condition to guarantee bounded solutions [Bel], [MaWi]. Also, certain attempts to approximate (4.48) by Mathieu's equation, by using either Fourier series expansions of F, or expansions with respect to the parameter σ, have failed and all led to physically unreasonable results. Nevertheless, numerical experiments of (4.48) by a Python code [Kats], for a wide range of values for the parameter σ show that the deviation between Bohmian and classical trajectories remains bounded for all time.



(a) $0 < \sigma \leq 0.1$

(b) $0.9 \leq \sigma \leq 1.15$

(c) $5 \leq \sigma \leq 50$

(d) $\sigma = 1000$

Figure. 4.2: *Deviation of trajectories for the harmonic oscillator*

CHAPTER 5

Discussion of the results

We have studied the quantum hydrodynamics of Gaussian wave packets travelling under the Schrödinger equation. We have constructed a process to identify the exact form of the wave packet depending on the potential that influences it and calculate the quantum potential it creates, along with the way its Bohmian trajectories diverge from its classical. We followed that process for the free particle case, the linear potential case and the quadratic potential case. In the free particle case, we saw that despite the absence of classical potential, quantum potential is produced and the particle diverges to infinity. It was also shown that the free particle and linear potential cases have the same Bohmian trajectory diversions, due to the second derivative of the potential being zero in both cases, and it may warrant further investigation. In the quadratic potential case, in order to find the form of the Bohmian trajectory divergence, we encountered Hill's equation. Exact solutions for this equation are very hard to find, so we tried to find out if we can get any information about the solution, such as boundness, without actually finding the solution itself. After a lot of research, we could not find any conditions that could prove anything useful, so we tried to rewrite the equation using Fourier series, due to $F(\tau)$ being periodic, which didn't produce any results. We then resorted in a numerical construction of the solution. It was then shown that the solutions were bounded for all time and are periodic for any value of the parameter $\sigma > 0$, except for $\sigma = 1$, where the solution remains constant. It could be interesting to further research for a theoretical way to prove the boundness of the solution. It would also be very interesting to investigate what happens for higher order potentials, such as cubic or anharmonic oscillation.

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Part III

Appendices & other background material

APPENDIX A

WKB method and geometrical optics

A.1 The WKB ansatz

In the *geometrical optics technique* [BLP] [Rau], one assumes an approximate WKB solution of the form

$$\psi^{\varepsilon}(x,t) = A^{\varepsilon}(x,t)e^{\frac{i}{\varepsilon}\Phi^{\varepsilon}(x,t)}\,, \tag{A.1}$$

where the amplitude A^{ε} and the phase Φ^{ε} are real valued functions, and they have the regular perturbation expansions

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

and

$$\Phi^{\varepsilon}(x,t) = \Phi(x,t) + \varepsilon \Phi_1(x,t) + \varepsilon^2 \Phi_2(x,t) + \ldots\ldots \tag{A.3}$$

Then, the derivatives of the wave function are given by

$$\partial_t \psi^{\varepsilon} = \Big(\partial_t A^{\varepsilon} + \frac{i}{\varepsilon} A^{\varepsilon}\partial_t \Phi^{\varepsilon}\Big)e^{\frac{i}{\varepsilon}\Phi^{\varepsilon}}, \tag{A.4}$$

$$\partial_x \psi^{\varepsilon} = \Big(\partial_x A^{\varepsilon} + \frac{i}{\varepsilon} A^{\varepsilon}\partial_x \Phi^{\varepsilon}\Big)e^{\frac{i}{\varepsilon}\Phi^{\varepsilon}}, \tag{A.5}$$

$$\partial_x \psi^{\varepsilon} = \partial_x\big(\partial_x \psi^{\varepsilon}\big) = \Big(\partial_x A^{\varepsilon} - \frac{1}{\varepsilon^2} A^{\varepsilon}\big(\partial_x \Phi^{\varepsilon}\big)^2 + \frac{1}{\varepsilon}\big(A^{\varepsilon}\partial_x^2 \Phi^{\varepsilon} + 2\partial_x \Phi^{\varepsilon}\partial_x A^{\varepsilon}\big)\Big)e^{\frac{i}{\varepsilon}\Phi^{\varepsilon}}\,. \tag{A.6}$$

By substituting $(A.4)\,,(A.5)\,,(A.6)$ into (1.1) we rewrite the Schrödinger equation in the form

$$i\varepsilon\big(\partial_t A^{\varepsilon} + \frac{i}{\varepsilon} A^{\varepsilon}\partial_t \Phi^{\varepsilon}\big) = -\frac{\varepsilon^2}{2}\Big(\partial_x A^{\varepsilon} - \frac{1}{\varepsilon^2} A^{\varepsilon}\big(\partial_x \Phi^{\varepsilon}\big)^2 + \frac{1}{\varepsilon}\big(A^{\varepsilon}\partial_x \Phi^{\varepsilon} + 2\partial_x \Phi^{\varepsilon}\partial_x A^{\varepsilon}\big)\Big) + V A^{\varepsilon}\,. \tag{A.7}$$

We further substitute the expansions $(A.2)\,,(A.3)$ into $(A.7)$, and we get the asymptotic equation

$$\varepsilon^0 A\Big(\partial_t \Phi + \frac{1}{2}\big(\partial_x \Phi\big)^2 + V\Big) - i\varepsilon\Big(\partial_t A + \frac{1}{2}\big(A\partial_x^2 \Phi + 2\partial_x \Phi \partial_x A\big)\Big) - \frac{\varepsilon^2}{2}\partial_x^2 A + \cdots = 0\,. \tag{A.8}$$

If we assume that A , Φ are smooth functions, equation $(A.8)$ is satisfied to order $O(\varepsilon^2)$, if the phase Φ satisfies the *Hamilton-Jacobi equation*

$$\partial_t \Phi + \frac{1}{2}\big(\partial_x \Phi\big)^2 + V = 0 \,, \tag{A.9}$$

and the amplitude A satisfies the *transport equation*

$$\partial_t A^2 + \partial_x \big(A^2 \partial_x \Phi\big) = 0 \,. \tag{A.10}$$

Remark. The equations $(A.9)$, $(A.10)$ 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]).

A.2 Hamiltonian system, Bicharacteristics 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

$$H(x,k) = \frac{1}{2}k^2 + V(x) \,, \tag{A.11}$$

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

$$\begin{cases} \frac{dx(t;q,p)}{dt} = k(t;q,p) \,, \\ \\ \frac{dk(t;q,p)}{dt} = -V'\big(x(t;q,p)\big) \,, \\ \\ x(0;q,p) = q, \qquad k(0;q,p) = p \,. \end{cases} \tag{A.12}$$

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

$$\begin{cases} \frac{d\bar{x}(t;q)}{dt} = \bar{k}(t;q) \,, \\ \\ \frac{d\bar{k}(t;q)}{dt} = -V'\big(\bar{x}(t;q)\big) \,, \\ \\ \bar{x}(0;q) = q \,, \;\; \bar{k}(0;q) = \mathrm{S}_0'(q) \,. \end{cases} \tag{A.13}$$

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

$$\begin{cases} \bar{x}(t;q) = \mathrm{S}_0'(q)t + q \,, \\ \\ \bar{k}(t;q) = \bar{k}(0;q) = \mathrm{S}_0'(q) \,, \end{cases} \tag{A.14}$$

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

$$\mathrm{J}(t;q) = \frac{\partial \bar{x}(t;q)}{\partial q}\ . \tag{A.15}$$

Whenever the Jacobian $(A.15)$ 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

$$\begin{cases} t = t_c(q)\ , \\ \\ \bar{x}_c(q) = \bar{x}\big(t_c(q);q\big)\ . \end{cases} \tag{A.16}$$

A.3 Hamilton-Jacobi and Transport Equations

A.3.1 Integration of Hamilton-Jacobi equation

By the identification $k = \partial_x\Phi(x,t)$, the initial value problem for the Hamilton-Jacobi equation $(A.9)$ is written in the form

$$\begin{cases} \partial_t\Phi(x,t) + H(x,\partial_x\Phi(x,t)) = 0\ , & x \in \mathbb{R}, t > 0\ , \\ \\ \Phi(x,t=0) = \mathrm{S}_0(x)\ . & x \in \mathbb{R}\ . \end{cases} \tag{A.17}$$

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 $(A.13)$, we have

$$\begin{aligned} \frac{d}{dt}\Phi\big(\bar{x}(t;q),t\big) &= \partial_t\Phi\big(\bar{x}(t;q),t\big) + \partial_x\Phi\big(\bar{x}(t;q),t\big)\frac{d\bar{x}(t;q)}{dt} \\ &= -\left(\frac{1}{2}\Big(\partial_x\Phi\big(\bar{x}(t;q),t\big)\Big)^2 + V\big(\bar{x}(t,q)\big)\right) + \partial_x\Phi\big(\bar{x}(t;q),t\big)\bar{k}(t;q) \\ &= -\frac{1}{2}\bar{k}^2(t;q) - V\big(\bar{x}(t;q)\big) + \bar{k}^2(t;q) \\ &= \frac{1}{2}\bar{k}^2(t;q) - V\big(\bar{x}(t;q)\big)\ . \end{aligned} \tag{A.18}$$

We integrate $(A.18)$ on the internal $(0,t)$, we immediately derive the phase

$$\Phi(\bar{x},t) = \mathrm{S}_0(q) + \int_0^t \left(\frac{1}{2}\bar{k}^2(\tau;q) - V\Big(\bar{x}(\tau;q)\Big)\right)d\tau\ . \tag{A.19}$$

A.4 Integration of the transport equation

We solve now the initial value problem for the transport equation

$$\begin{cases} \partial_t \mathrm{A}^2(x,t) + \partial_x\big(\mathrm{A}^2(x,t)\partial_x\Phi(x,t)\big) = 0, \quad x \in \mathbb{R},\ t > 0\ , \\ \\ \mathrm{A}(x,t=0) = \mathrm{A}_0(x)\ ,\ x \in \mathbb{R}\ . \end{cases} \tag{A.20}$$

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

$$\begin{aligned} \frac{d}{dt}\ln \mathrm{A}^2\big(\bar{x}(t,\alpha),t\big) &= \frac{1}{\mathrm{A}^2\big(\bar{x}(t,\alpha),t\big)}\frac{d}{dt}\mathrm{A}^2\big(\bar{x}(t,\alpha),t\big) \\ &= \frac{\big(\partial_t \mathrm{A}^2 + \partial_x \mathrm{A}^2 \partial_x \Phi\big)\big(\bar{x}(t,\alpha),t\big)}{\mathrm{A}^2\big(\bar{x}(t,\alpha),t\big)} \\ &= -\partial_x^2\Phi\big(\bar{x}(t,\alpha),t\big)\ . \end{aligned} \tag{A.21}$$

Then, by Liouville's formula for the equation

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

we get

$$\frac{d}{dt}\ln \mathrm{J}(t,q) = \partial_x \bar{k}(t,q) = \partial_x\Big(\partial_x\Phi\big(\bar{x}(t,q),t\big)\Big) = \partial_x^2\Phi\big(\bar{x}(t,q),t\big)\ . \tag{A.22}$$

Thus, we obtain

$$\frac{d}{dt}\ln \mathrm{A}^2\big(\bar{x}(t,\alpha),t\big) = -\frac{d}{dt}\ln \mathrm{J}(t,q)\ . \tag{A.23}$$

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

$$\mathrm{A}\big(\bar{x}(t,q),t\big) = \frac{\mathrm{A}_0(q)}{\sqrt{\mathrm{J}(t,q)}}\ . \tag{A.24}$$

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 $(A.24)$ 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).