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Beyond WKB quantum corrections to Hamilton–Jacobi theory

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Abstract

In this paper, we develop quantum mechanics of quasi-one-dimensional systems upon the framework of the quantum-mechanical Hamilton–Jacobi theory. We will show that the Schrödinger point of view and the Hamilton–Jacobi point of view are fully equivalent in their description of physical systems, but differ in their descriptive manner. As a main result of this, a wavefunction in Hamilton–Jacobi theory can be decomposed into travelling waves in any point in space, not only asymptotically. Using the quasi-linearization technique, we derive quantum correction functions in every order of $\hbar$. The quantum correction functions will remove the turning-point singularity that plagues the WKB-series expansion already in zeroth order and thus provide an extremely good approximation to the full solution of the Schrödinger equation. In the language of quantum action it is also possible to elegantly solve the connection problem without asymptotic approximations. The use of quantum action further allows us to derive an equation by which the Maslov index is directly calculable without any approximations. Stationary quantum trajectories will also be considered and thoroughly discussed.

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1. Introduction

It must have been a subconscious path that guided Schrödinger to the derivation of his famous equation in the early days of 1926 [1]. Schrödinger started with the classical Hamilton–Jacobi equation, transformed the classical action function s by $s = -\mathrm{i}\hbar \ln[\Psi]$, performed an adventurous variational calculation on the Hamilton integral and arrived at his celebrated result

$$\Psi''(x) + p^2(x)\Psi(x) = 0, \qquad p(x) = \sqrt{2m(E - U(x))}/\hbar. \tag{1}$$

Several attempts have since been made to relate the quantum mechanics perfectly described by (1) to quantities that are known from classical mechanics, action and momentum;

these attempts are twofold. The first one was taken already by Madelung [2] in 1926. Madelung introduced the polar wavefunction, $\Psi(x) = A(x)\exp[\mathrm{i}S_{\mathrm{M}}(x)/\hbar]$, where $S_{\mathrm{M}}(x)$ is the Madelung action function and both $A, S_{\mathrm{M}}(x)$ are real. Madelung's way was further taken by Bohm [3] in his attempt to build a causal quantum theory. But the initial separation of the real and imaginary parts of the wavefunction leads to very complicated equations for amplitude and phase and will not be pursued here. For exhaustive information on the Madelung–de Broglie–Bohm theory see [4, 5] and for modern application [6]. The work of Floyd [7] especially pursued the theory of the stationary Hamilton–Jacobi theory with quantum potentials, while Faraggi and Matone [8] worked out some fundamental ideas on the geometrical meaning of the quantum potential.

The second way is to initially keep the real and imaginary parts of the quantum action function together, $\Psi(x) = \exp[\mathrm{i}S(x)/\hbar]$, leading to the Hamilton–Jacobi equation of quantum mechanics,

$$(S'(x))^2 - \mathrm{i}\hbar S''(x) = p^2(x). \tag{2}$$

Also in 1926, Wentzel, Kramers and Brillouin [9], starting from (2), proposed an expansion of the full quantum action function $S(x,\hbar)$ by small values of $\hbar$, which finally leads to the classical action, perturbed by small corrections of order $\hbar$. The WKB theory works surprisingly well, but it breaks down in the vicinity of *quantal* regions, where the WKB wavefunction is plagued by singularities. For an exhaustive review on this topic see [10] and references therein.

Various methods, most of them are reviewed in [11], have been developed to improve the WKB theory. The most elaborated among these are the Fröman–Fröman series [12] and the use of the quasi-linearization method by Raghunathan and Vasudevan [13]. The method of quasi-linearization has the advantage that it initially does not rely on the existence of a small expansion parameter $\hbar$ in our case. Quasi-linearization, as applied to quantum mechanics in [13], is the starting point of our paper. We are going to develop the use of quasi-linearization techniques from a systematic and physically reasonable point of view, which was neglected in [13]. The systematic use of this technique will lead us to the definition of a quantum correction function. This is a function that describes all quantum effects of a physical system.

2. Quantum correction functions

By introducing a local gradient field, which can easily be identified with the local quantum momentum,

$$S(x) = \int^x P(x)\,\mathrm{d}x \leftrightarrow P(x) = S'(x), \tag{3}$$

the Hamilton–Jacobi equation (2) can be cast into

$$P^2(x) - \mathrm{i}\hbar P'(x) = p^2(x). \tag{4}$$

To be able to distinguish between the influence of classical mechanics and quantum mechanics on the behaviour of a physical system, we propose that the full quantum momentum field $P(x)$ can be decomposed into its classical part and a contribution arising purely by quantum effects. We set

$$P(x) = p(x) + Q(x). \tag{5}$$

The function $Q(x)$ is called a *quantum correction function*, because it describes purely quantum effects and thus corrects the behaviour of the classical movement, governed by the classical momentum $p(x)$. More precisely, the function $Q(x)$ describes the difference between the full quantum momentum $P(x)$ and its classical contribution $p(x)$,

$$Q(x) = P(x) - p(x). \tag{6}$$

It can be concluded easily that $Q(x)$ tends to zero in regions where the motion is known to be purely classical. We want to emphasize that the introduction of the quantum correction function $Q(x)$ does *not* change the constants of motion, their number is the same as in the classical case. By assuming multidimensionality at first, one can easily show that the conditions for separability of (2) and (4) are the same as in the classical case. Thus the classical number for the constants of motion is conserved, as it should.

To derive an analytic expression for the quantum correction function $Q(x)$, we insert (5) into the Hamiltonian–Jacobi equation (4) and find an differential equation for $Q(x)$:

$$Q(x)\{2p(x) + Q(x)\} - \mathrm{i}\hbar\{p'(x) + Q'(x)\} = 0. \tag{7}$$

This nonlinear first-order equation can be formally integrated to yield a self-consistent formula for the quantum correction function $Q(x)$,

$$Q(x) = -\exp\left[-\frac{\mathrm{i}}{\hbar}\int^{x}\{2p(y) + Q(y)\}\,\mathrm{d}y\right]\int^{x} p'(y)\exp\left[\frac{\mathrm{i}}{\hbar}\int^{y}\{2p(z) + Q(z)\}\,\mathrm{d}z\right]\mathrm{d}y. \tag{8}$$

We emphasize that this expression for $Q(x)$ is exact; so far, no approximation has been made. In the following, we will examine the structure of this expression and formulate a systematic perturbational approach. This perturbational approach does not, as it is usually done for semiclassical questions, start initially with the expansion in terms of $\hbar$, it will consist of quantum correction functions that contain every order in $\hbar$. This will open a more general sight onto the behaviour of physical systems near their semiclassical limit.

2.1. Perturbation theory

The main reason to examine quantum-mechanical systems in Hamilton–Jacobi formulation is to clearly distinguish between classical and quantum behaviour. As we will see below, the semiclassical limit of Hamilton–Jacobi quantum mechanics is open to perturbation theory, while its full quantum description belongs to the non-perturbative regime. The main result of the following subsection is, that in the one-dimensional case, we are able to introduce an operator formalism, which is, in its structure, closely related to the well-known Dirac or interaction representation. Writing equation (8) in a more operational sense, we can set up a formalism for the perturbational expansion. The central quantity of this operator formalism is given by

$$Q(x) = \exp\left[-\frac{\mathrm{i}}{\hbar}W(x)\right]\hat{\mathbf{Q}}(x)\exp\left[\frac{\mathrm{i}}{\hbar}W(x)\right], \tag{9}$$

where the quantum action function is given by

$$S(x) = s(x) + W(x), \tag{10}$$

$s(x)$ is the classical action and $W(x)$ is the quantum action correction function. The structure of (9) enables us to make use of the Baker–Hausdorff identity, which allows a formal expansion,

$$\begin{aligned} Q(x) &= \exp\left[-\frac{\mathrm{i}}{\hbar}W(x)\right]\hat{\mathbf{Q}}(x)\exp\left[\frac{\mathrm{i}}{\hbar}W(x)\right] \\ &= Q_0(x) - \frac{\mathrm{i}}{\hbar}[W(x), \hat{\mathbf{Q}}(x)] + \frac{1}{2}\left(\frac{\mathrm{i}}{\hbar}\right)^2[W(x), [W(x), \hat{\mathbf{Q}}(x)]] + \cdots \\ &= Q_0(x) + Q_1(x) + Q_2(x) + \cdots. \end{aligned} \tag{11}$$

The zeroth-order correction function $Q_0(x)$ comes from

$$Q_0(x) = \hat{\mathbf{Q}}(x)\cdot 1 = -\exp\left[-\frac{\mathrm{i}}{\hbar}2s(x)\right]\int^{x} p'(y)\exp\left[\frac{\mathrm{i}}{\hbar}2s(y)\right]\mathrm{d}y. \tag{12}$$

This corresponds to the zeroth iteration of equation (9), where the action correction $W(x)$ is chosen zero.

2.2. Convergence properties

The convergence behaviour of our perturbation series depends crucially on its key quantity, the function $Q_0(x)$. The whole perturbation series is built on this zeroth-order quantum correction function, and thus the behaviour of this function will influence the behaviour of the perturbation series. The question we have to ask must be, if there are singularities around classical turning points, which plague the WKB theory. Anticipating the answer, we can state: the function $Q_0(x)$ is regular in the vicinity of classical turning points x_t, if and only if the potential function $U(x)$ is regular there. The examination now follows.

We want to examine, if the integral, which determines the function $Q_0(x)$, possesses upper or lower bounds. We have

$$Q_0(x) = -\exp\left[\mathrm{i}2s(x)\right] \int^x p'(y) \exp\left[\mathrm{i}2s(y)\right] \mathrm{d}y. \tag{13}$$

Since we are interested in the behaviour of $Q_0(x)$ in the vicinity of a classical turning point, we expand the integrand around the classical turning point:

$$\begin{aligned} p'(x) &= -\frac{U'(x)}{2\sqrt{k^2 - U(x)}} \approx -\frac{U'(x_t) + U''(x_t)(x - x_t)}{2\sqrt{-U'(x_t)(x - x_t)}}, \\ s(x) &= \int^x \sqrt{k^2 - U(x)}\, \mathrm{d}x \approx \frac{2}{3}\sqrt{-U'(x_t)}(x - x_t)^{3/2}. \end{aligned} \tag{14}$$

This approximation is suitable, because the function $p'(x)$, which is the origin of the turning-point singularity, is approximately zero almost everywhere, except the turning-point region. Thus, the main contribution to the integral comes directly from the turning-point region. Inserting the approximate quantities and performing the integral, we get the following estimate:

$$\lim_{x \to x_t} |Q_0(x)| \approx \left| \frac{1}{6^{2/3}} \left(U'(x_t)\right)^{\frac{1}{3}} \Gamma\left[\frac{1}{3}\right] + \frac{U''(x_t)}{4U'(x_t)} \right|. \tag{15}$$

We clearly see, that near the turning point the behaviour of $Q_0(x)$ depends directly on the behaviour of the potential function $U(x)$. When $U(x)$ is regular at x_t, which is the case for all potentials that locally can be represented by powers $x^\alpha, \alpha > 0$, the quantum correction function itself is regular and finite. When $U(x)$ is unbounded near x_t, which is the case for potentials, that locally can be represented by inverse powers $x^{-\alpha}, \alpha > 0$, then the quantum correction function will diverge, too.

From this it follows that in the vicinity of a classical turning point the full action function $S(x)$ is strongly influenced by its quantum contribution $W(x)$. Far away from the classical turning point, in regions where the quantum correction function $Q(x)$ has vanished, the action of the system is purely given by the classical action function $s(x)$. In the cases where the potential has become a constant, the classical action function is then naturally given by $s(x) \sim kx$, where k is the suitable wave vector (see, e.g., [10]).

From a more mathematical point of view, Mandelzveig [14] has shown that expressions such as (9) converge *quadratically*. Physically spoken, quadratical convergence means that the zeroth iterate $Q_0(x)$ is already very close to the exact result $Q(x)$, such that qualitatively the whole quantum-mechanical behaviour of a system is to be described by the zeroth iterate $Q_0(x)$.

2.3. The order of the perturbing terms

From the perturbation series (11), the order in $\hbar$ is not easily visible. We have seen in (11) that the full quantum momentum can be expressed as a series

$$P(x) = p(x) + \sum_{\mu=0}^{\infty} Q_\mu(x). \tag{16}$$

On the other hand, it is known that the full quantum momentum can be expanded in power of $\hbar$, when $\hbar$ is small compared to the classical action function,

$$P(x) = p(x) + \sum_{\nu=1}^{\infty} \hbar^\nu P_\nu(x). \tag{17}$$

The crucial question now is, how these two series are related to each other. To get more insight into this question, we start with the self-consistent expression (9) for $Q(x)$. Due to self-consistency, the correction function $Q(x)$ is a function of *all* orders of $\hbar$. To see this more clearly, we can formally put the indices μ, ν together and obtain

$$Q(x) = \sum_{\mu=0}^{\infty} Q_\mu(x) = \sum_{\mu=0}^{\infty}\sum_{\nu=1}^{\infty} \hbar^\nu Q_{\mu\nu}(x), \qquad Q_\mu(x) = \sum_{\nu=1}^{\infty} \hbar^\nu Q_{\mu\nu}(x). \tag{18}$$

This means that every order of quantum correction functions carries all orders of $\hbar$, as stated above. This fact will be demonstrated in the following subsection, where the power series in $\hbar$ is calculated directly from the quantum correction functions.

2.4. Derivation of the WKB regime

After these formal preparations, we will calculate the power series in $\hbar$. One of the most interesting results of this calculation will be a reason for the bad convergence of the WKB series.

The WKB theory follows from the assumption that the solutions of the Hamilton–Jacobi equation can be represented as power series in $\hbar$,

$$S(x) = s(x) + \sum_{\nu=1}^{\infty} \hbar^\nu S_\nu(x), \qquad P(x) = p(x) + \sum_{\nu=1}^{\infty} \hbar^\nu P_\nu(x). \tag{19}$$

When these ansätze are inserted into the Hamilton–Jacobi equations (2) and (4), there arises an infinite hierarchy of equations, which can only be solved by successive approximation. Breaking this infinite hierarchy after the first order yields the familiar WKB result for the wavefunction. But the expansion in powers of $\hbar$ is plagued by singularities around the classical turning points, and the strength of these singularities increases by every order in $\hbar$. This is not the case, when the series expansion is derived from the quantum correction functions, because their expansion in powers of $\hbar$ will create residual terms of higher order in $\hbar$, which will catch the divergencies and result finite expressions as a whole.

Technically, the expansion can be set up as follows. By the use of the auxiliary identity $1 = p(x)/p(x)$, we get for the zeroth order

$$\begin{aligned} Q_0(x) &= -\exp\left[-\frac{\mathrm{i}}{\hbar}2s(x)\right]\int^x p'(y)\exp\left[\frac{\mathrm{i}}{\hbar}2s(y)\right]\mathrm{d}y \\ &= -\exp\left[-\frac{\mathrm{i}}{\hbar}2s(x)\right]\int^x p'(y)\left(\frac{p(y)}{p(y)}\right)\exp\left[\frac{\mathrm{i}}{\hbar}2s(y)\right]\mathrm{d}y. \end{aligned} \tag{20}$$

Performing an integration by parts, one gets

$$Q_0(x) = \hbar\frac{\mathrm{i}}{2}\frac{p'(x)}{p(x)} + \hbar\frac{\mathrm{i}}{2}\exp\left[-\frac{\mathrm{i}}{\hbar}2s(x)\right]\int^x \mathrm{d}z\left(\frac{p'}{p}\right)'(z)\exp\left[\frac{\mathrm{i}}{\hbar}2s(z)\right]. \tag{21}$$

Using the auxiliary identity once again and integrating by parts yields

$$Q_0(x) = \hbar\frac{\mathrm{i}}{2}\frac{p'(x)}{p(x)} - \hbar^2\frac{1}{4}\frac{p(x)p''(x) - (p'(x))^2}{p^3(x)} + R_{0,3}(x). \tag{22}$$

We observe the following facts: the term proportional to $\hbar$ is precisely the first-order series expansion following from the WKB theory; the following term is of order $\hbar^2$, and does not contribute to the first order in $\hbar$. The residual term denoted by $R_{\mu=0,\nu=3}(x)$ carries only powers of $\hbar$ equal to or larger than $\nu = 3$. Such a residual term is not known in WKB theory; it is lost by initially assuming the power expansion in terms of $\hbar$.

Up to now, we have shown that the zeroth-order quantum correction leads to the correct WKB-term first order in $\hbar$,

$$\hbar P_1(x) = Q_{0,1}(x) = \hbar\frac{\mathrm{i}}{2}\frac{p'(x)}{p(x)}. \tag{23}$$

The second-order expansion in WKB theory gives

$$\hbar^2 P_2(x) = -\hbar^2\frac{1}{4}\frac{p(x)p''(x) - (p'(x))^2}{p^3(x)} + \hbar^2\frac{1}{8}\frac{(p'(x))^2}{p^3(x)}. \tag{24}$$

The first term has already been obtained by the second integration by parts of $Q_0(x)$. Further integrations by parts of $R_{0,3}(x)$ in the same manner would not lead to the required second term; it can only be calculated by expanding $Q_1(x)$ into powers of $\hbar$. The perturbational expression for $Q_1(x)$ as calculated above (11) is

$$Q_1(x) = -\frac{\mathrm{i}}{\hbar}\left[\int^x Q(z)\,\mathrm{d}z, \hat{\mathbf{Q}}(x)\right] = -\frac{\mathrm{i}}{\hbar}\left[\hbar\int^x Q_{0,1}(z)\,\mathrm{d}z, \hat{\mathbf{Q}}(x)\right]. \tag{25}$$

The first integration by parts cancels, such that only terms of order $\mathcal{O}(\hbar^2)$ remain,

$$\begin{aligned} Q_1(x) &= -\hbar\frac{1}{2}\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}2s(x)}\int^x \mathrm{d}z\frac{p'(z)}{p(z)}Q_{0,1}(z)\,\mathrm{e}^{\frac{\mathrm{i}}{\hbar}2s(z)} - \left[\int^x Q_{0,1}(z)\,\mathrm{d}z, \hat{\mathbf{R}}_{0,3}(x)\right] \\ &= -\hbar^2\frac{\mathrm{i}}{4}\frac{p'(x)}{p^2(x)}Q_{0,1}(x) + R_{1,3}(x) - \left[\int^x Q_{0,1}(z)\,\mathrm{d}z, \hat{\mathbf{R}}_{0,3}(x)\right]. \end{aligned} \tag{26}$$

We have introduced a residual operator $\hat{\mathbf{R}}_{\mu,\nu}$ for denoting terms of higher order $\hbar$ remaining under the integral. The first order in $\hbar$ is already known from above, $Q_{0,1}(x) = \frac{\mathrm{i}}{2}\frac{p'(x)}{p(x)}$, leading to the first term of the desired WKB expression,

$$Q_1(x) = Q_{1,2}(x) + \cdots = \hbar^2\frac{1}{8}\frac{(p'(x))^2}{p^3(x)} + \cdots. \tag{27}$$

With that, we obtain

$$\begin{aligned} &P_1(x) = Q_{0,1}(x), \\ &P_2(x) = Q_{0,2}(x) + Q_{1,2}(x), \\ &\cdots\cdots \end{aligned} \tag{28}$$

The residual terms $R_{\mu\nu}(x)$ and $\hat{\mathbf{R}}_{\mu\nu}(x)$ carry only higher orders in $\hbar$.

With this, rather cumbersome, procedure we could show, how all orders of the WKB series can be obtained, at least in principle. It further clarifies the fidelity of the quantum correction functions: $Q_0(x)$ is exact to the first order in $\hbar$, $Q_0(x) + Q_1(x)$ is exact to the second order in $\hbar$ and so on. Keeping the WKB form, we can write the quantum-mechanical momentum as

$$P(x) = p(x) + \sum_{\nu=1}^{N} \hbar^{\nu} P_{\nu}(x) + \sum_{\mu=0}^{\infty} \sum_{\nu=N+1}^{\infty} \mathcal{R}_{\mu\nu}(x), \tag{29}$$

where in $\mathcal{R}(x)$ we have subsummized all residual terms. The number N gives the order in $\hbar$. The residual terms cannot be obtained when the WKB-series expansion is set initially. The residual terms result from partially integrating the nonsingular expression for the quantum correction function $Q(x)$, but a nonsingular expression will remain nonsingular. The procedure of partial integration splits the nonsingular quantum correction function into a singular WKB-term and a singular residual term. Both singularities kept together will give a nonsingular function, but omitting the residual terms, as WKB theory does, will give a badly converging, singular power series in $\hbar$.

3. The construction of the wavefunction

The key to the construction of the wavefunction is the action integral that depends on the direction of integration. In a two-turning-point system, we have the choice to integrate from the left (x_1) to the right (x_2) or vice versa. We have reserved a whole section to this problem, because its solution is not as easy as it might look at first.

We begin with the wavefunction, that is obtained by integrating from the left to the right, $x_1 \to x_2$. We find, in a trigonometric fashion,

$$\Psi(x) = \exp\left[-\int_{x_1}^{x} \mathrm{Im}Q(x')\,\mathrm{d}x'\right] \cos\left[\int_{x_1}^{x} \left(p(x') + \mathrm{Re}Q(x')\right)\,\mathrm{d}x' - \frac{\phi_{\rightarrow}}{2}\right]. \tag{30}$$

The arrow index of the reflection phase indicates that the direction of integration here was chosen as $x_1 \to x_2$. To construct this wavefunction, we have made the following choice for the quantum momentum function:

$$P(x) = p(x) + \mathrm{Re}Q(x) + \mathrm{i}\,\mathrm{Im}Q(x). \tag{31}$$

The easiest way to construct the reverse direction is to introduce a parity transformation by the operator $\hat{\mathbf{T}}_{\mathbf{P}}$, which performs an axialsymmetric transformation. The position of this axis will be the minimum of the potential—the potential itself may be of unsymmetric shape, the minimum is the only condition—that any two-turning-point system will possess. We want to know what a wave, which starts at x_1 would look like, when it starts at x_2,

$$\hat{\mathbf{T}}_{\mathbf{P}} \exp\left[\mathrm{i}\int_{x_1}^{x} (p(x') + \mathrm{Re}Q(x') + \mathrm{i}\,\mathrm{Im}Q(x'))\,\mathrm{d}x'\right] = \exp\left[\mathrm{i}\int_{x_2}^{x} (p(x') + \mathrm{Re}Q(x) - \mathrm{i}\,\mathrm{Im}Q(x'))\,\mathrm{d}x'\right]. \tag{32}$$

The sign of the imaginary momentum function has changed. This is due to the fact that the real parts of the quantum momentum are even, the imaginary part is an odd function with respect to the minimum of the potential. This can be deduced from (9) by inspection. Thus, when a parity transform with respect to this minimum is applied, the sign of the imaginary

part must be changed. Without this fact, a consistent construction of a wavefunction for the direction of integration $x_1 \leftarrow x_2$ is not possible. We finally obtain

$$\Psi(x) = \exp\left[\int_{x_2}^{x} \mathrm{Im}Q(x')\,\mathrm{d}x'\right]\cos\left[\int_{x_2}^{x}(p(x')+\mathrm{Re}Q(x'))\,\mathrm{d}x' - \frac{\phi_{\leftarrow}}{2}\right]$$
$$= \exp\left[-\int_{x}^{x_2} \mathrm{Im}Q(x')\,\mathrm{d}x'\right]\cos\left[-\int_{x}^{x_2}(p(x')+\mathrm{Re}Q(x'))\,\mathrm{d}x' - \frac{\phi_{\leftarrow}}{2}\right]. \tag{33}$$

4. Soft boundary problems and quantization

In the framework of Hamilton–Jacobi theory, soft boundary problems arise, because the space is separated into classically allowed and classically forbidden regions. By solving the appropriate Hamilton–Jacobi equations, a wavefunction Ψ_i for each of these regions is known. The boundary value problem is to match all these wavefunctions to obtain a wavefunction Ψ defined on the whole space. This boundary value problem is also known as the connection problem, see, e.g., [11]. In the Schrödinger point of view the connection problem

$$\Psi_1(x) \leftrightarrow \Psi_2(x) \leftrightarrow \Psi_3(x) \tag{34}$$

is a formidable task and will, except some few solvable examples, remain unsolved in general. In the Hamilton–Jacobi point of view, we can express the wavefunctions as exponentials, and the connection problem becomes easily treatable on the level of trigonometric and exponential functions,

$$\exp[-S_1(x)] \leftrightarrow \exp[-\mathrm{Im}S_2(x)]\cos\left[\mathrm{Re}S_2(x) - \frac{\phi}{2}\right] \leftrightarrow \exp[-S_3(x)]. \tag{35}$$

The reflection phase ϕ solves the connection problem and with ϕ the wavefunction can be defined on the whole space.

The points where the wavefunctions of different spatial regions have to be matched are the classical turning points. The boundary value problem, e.g.,

$$\frac{\partial}{\partial x}\ln[\Psi_2(x)]\bigg|_{x=x_2} = \frac{\partial}{\partial x}\ln[\Psi_3(x)]\bigg|_{x=x_2}, \tag{36}$$

is called a soft boundary problem, because it is neither a Dirichlet nor a Neumann boundary problem, but a mixture of both. Writing (36) in the spirit of (35), we obtain

$$-\mathrm{Im}Q_2(x_2) - \mathrm{Re}Q_2(x_2)\tan\left[\int_{x_1}^{x_2}(p_2(x')+\mathrm{Re}Q_2(x'))\,\mathrm{d}x' - \frac{\phi_{\rightarrow}}{2}\right] = -Q_3(x_2). \tag{37}$$

From this, we obtain the reflection phase

$$\phi_{\rightarrow} = 2\arctan\left[\frac{\mathrm{Im}Q_2(x_2) - Q_3(x_2)}{\mathrm{Re}Q_2(x_2)}\right] + 2\int_{x_1}^{x_2}(p_2(x')+\mathrm{Re}Q_2(x'))\,\mathrm{d}x'. \tag{38}$$

For the reverse direction, we similarly find

$$\phi_{\leftarrow} = 2\arctan\left[\frac{\mathrm{Im}Q_2(x_1) + Q_1(x_1)}{\mathrm{Re}Q_2(x_1)}\right] - 2\int_{x_1}^{x_2}(p_2(x')+\mathrm{Re}Q_2(x'))\,\mathrm{d}x'. \tag{39}$$

The reflection phases, by their dependence on the turning points, are functions of energy.

Knowing the reflection phases, we can easily derive the quantization law by the argument that both directions of integration must give the same wavefunction. The phases of this

wavefunctions may only differ by $n\pi$. From this, we get

$$\int_{x_1}^{x_2} \mathrm{Re}\, P_2(x')\,\mathrm{d}x' - \frac{\phi_{\rightarrow} + \phi_{\leftarrow}}{2} = n\pi. \tag{40}$$

Note that by (38) and (39) the action integrals cancel each other in the sum $\phi_{\rightarrow} + \phi_{\leftarrow}$. To make contact with the usual Bohr–Sommerfeld rule, we rewrite (40) and introduce the Maslov index μ_ϕ

$$\begin{aligned} &\int_{x_1}^{x_2} p_2(x')\,\mathrm{d}x' = \pi\left(n + \frac{\mu_\phi}{4}\right), \\ &\mu_\phi = \frac{4}{\pi}\left(\frac{\phi_{\rightarrow} + \phi_{\leftarrow}}{2} - \int_{x_1}^{x_2} \mathrm{Re}\, Q_2(x')\,\mathrm{d}x'\right). \end{aligned} \tag{41}$$

With (41) the Maslov index of a physical system is directly calculable by knowledge of the quantum correction function. This is a very valuable result, because quantization in the Hamilton–Jacobi point of view means just to calculate (41) to obtain the energy levels. There is no need to orthonormalize the wavefunctions to find the energy levels, when calculated by (41). The theory of Hilbert spaces ensures that the wavefunctions corresponding to eigenvalues of the underlying problem are already orthonormal.

By (38) and (39), we can examine another important property of the reflection phases. They are divided into two parts, one gauge dependent and the other gauge invariant,

$$\phi = \phi^{\mathrm{g}} + \phi^{\mathrm{inv}}, \tag{42}$$

Inspection of (38) and (39), in combination with (30) and (33) shows that the lower bound of integration does not necessarily have to be a turning point. Depending on the direction of integration, which has to be defined at first, the lower bound serves as a point of reference and can be chosen arbitrarily as any point lying between the two turning points. The choice of the lower bound must leave the wavefunction invariant. This is ensured by the gauge-dependent part of the reflection phase, e.g.,

$$\phi^{\mathrm{g}}_{\rightarrow} = 2\int_{x_{\mathrm{ref}}}^{x_2} (p_2(x') + \mathrm{Re}\, Q_2(x'))\,\mathrm{d}x'. \tag{43}$$

The gauge-invariant part is thus given by, e.g.,

$$\phi^{\mathrm{inv}}_{\rightarrow} = 2\arctan\left[\frac{\mathrm{Im}\, Q_2(x_2) - Q_3(x_2)}{\mathrm{Re}\, Q_2(x_2)}\right]. \tag{44}$$

5. Quantum trajectories

The topic of quantum trajectories is often discussed by introducing a quantum potential and a quantum force. We refuse the introduction of those quantities, because to our opinion they are somewhat misleading. The so called quantum potential is not a potential function as classical potentials are, but depends on the real part of the reduced quantum-mechanical action function, so does the quantum force. From this point of view, one anyway has to solve the Hamilton–Jacobi equation at first and calculate the quantum potential afterwards, which makes the introduction of a quantum potential gratuitous (for the here-discussed stationary theory). There is another crucial point, that leads us to reject the concept of a quantum potential, because, as we will show below, the classical relation between momentum and velocity does not hold within the framework of the quantum-mechanical Hamilton–Jacobi theory. The trajectory has thus to be derived from the quantum-mechanical action function directly. From this trajectory, by time derivatives, it would in principle be possible to construct

a Lagrangian or Newton's equation of motion, but such attempts are, again, gratuitous to our opinion.

The use of the stationary Hamilton–Jacobi equation describes isoenergetic dynamics, meaning that motion takes place on a energy shell in phase space. The presence of quantum-mechanical behaviour has no effect on the energy shell itself. This can be demonstrated by writing the classical and quantum-mechanical Hamiltonians as

$$\mathcal{H}_{\mathrm{cl}} = \frac{p^2}{2m} + U(x), \qquad \mathcal{H}_{\mathrm{qm}} = \frac{P^2}{2m} - \frac{\mathrm{i}\hbar}{2m}\frac{\partial}{\partial x}P + U(x), \tag{45}$$

and comparing them:

$$\mathcal{H}_{\mathrm{qm}} - \mathcal{H}_{\mathrm{cl}} = \delta\mathcal{H}. \tag{46}$$

If in (46) $\delta\mathcal{H}$ is zero, the energy of quantum and classical motion is constrained to the same energy shell, quantum and classical motion are isoenergetic to each other. The employment of quasilinearization $P = p + Q$ naturally fulfils $\delta\mathcal{H} = 0$ because

$$\mathcal{H}_{\mathrm{qm}} = \mathcal{H}_{\mathrm{cl}}, \tag{47}$$

$$0 = 2pQ + Q^2 - \mathrm{i}\hbar\frac{\partial}{\partial x}(p + Q). \tag{48}$$

The presence of the quantum momentum corrections thus has no effect on the energy of the system; they only change the dynamical flow on the energy shell. For the dynamics that means, that the time the motion between two points takes is changed. In the light of (48) it becomes clear how misleading the introduction of concepts like quantum potentials is, because a genuine potential function should of course change the total energy of the system.

The presence of a quantum momentum correction leads to a different trajectory,

$$x_{\mathrm{q}}(t) = x_{\mathrm{cl}}(t) + x_{\mathrm{qm}}(t), \tag{49}$$

where the total motion is divided into a purely classical and a purely quantum-mechanical part. Naively one would think that from (49) it immediately follows that

$$m\frac{\mathrm{d}x_{\mathrm{q}}(t)}{\mathrm{d}t} = p(x) + \mathrm{Re}Q(x), \tag{50}$$

which, as we will show now, is not true. In the classical mechanics, the trajectory equation, see equation (54), and the velocity–momentum relation are equal. We have

$$\mathrm{d}t = \mathrm{d}x\frac{\partial p(x)}{\partial E} \rightarrow \frac{\mathrm{d}x}{\mathrm{d}t} = \left(\frac{\partial p(x)}{\partial E}\right)^{-1} = \left(\frac{m}{p(x)}\right)^{-1} = \frac{p(x)}{m}. \tag{51}$$

In quantum mechanics, the quantum momentum correction breaks this equality, leading to

$$\frac{\mathrm{d}x}{\mathrm{d}t} = \left(\frac{\partial p(x)}{\partial E} + \frac{\partial\,\mathrm{Re}Q(x)}{\partial E}\right)^{-1} \neq \frac{1}{m}\left(p(x) + \mathrm{Re}Q(x)\right). \tag{52}$$

It can easily be seen that the naive assumption (50) leads to an obviously wrong result. See [16, 17] for statements to the same effect.

The necessary theoretical tool to calculate a trajectory is already known from the classical mechanics. As there, we start with the action function

$$\mathrm{Re}S = \int_{x_{\mathrm{ref}}}^{x_2} \mathrm{d}x\left(p(x) + \mathrm{Re}Q(x)\right) - E\left(t - t_0\right). \tag{53}$$

Employing the Jacobi connection, which is the same as demanding the phase of the wavefunction to be stationary, it follows that

$$t - t_0 = \mathrm{Re}\frac{\partial S}{\partial E}, \tag{54}$$

which we will call the trajectory equation. The use of the Jacobi connection is a natural consequence of the Hamilton–Jacobi theory. Theoretically, it is very well founded and will give the right trajectory for any given action function. Thus, we dwell on a very safe terrain, whereas (50) is not more than an assumption.

It is common knowledge that a standing wave, e.g. a bound state, has a current density of zero, and thus contains no observable motion. This is certainly true in cases where only the wavefunction Ψ is known. The use of the quantum action function S instead allows a decomposition into running waves, which certainly possess a dynamical interpretation. This dynamical interpretation allows us to connect the motion of a quantum particle with a causal picture. From (54) we get the running time differences between the classical and quantum motion moving from an arbitrarily chosen point to a turning point and back,

$$\begin{aligned}\Delta t_{\rightarrow} &= \int_{x_{\mathrm{ref}}}^{x_2} \mathrm{d}x \left(\frac{\partial p(x)}{\partial E} - \frac{\partial \operatorname{Re} P(x)}{\partial E} \right), \\ \Delta t_{\leftarrow} &= -\int_{x_{\mathrm{ref}}}^{x_2} \mathrm{d}x \left(\frac{\partial p(x)}{\partial E} - \frac{\partial \operatorname{Re} P(x)}{\partial E} \right).\end{aligned} \tag{55}$$

From (55), we obtain the total time shift between the quantum and classical motion

$$\Delta t = \Delta t_{\rightarrow} - \Delta t_{\leftarrow} = -2 \int_{x_{\mathrm{ref}}}^{x_2} \mathrm{d}x \frac{\partial \operatorname{Re} Q(x)}{\partial E}. \tag{56}$$

The total time shift is a positive function of energy and a consequence of the isoenergeticity. Its meaning is as follows: the quantum particle moves with a larger local momentum as the classical particle does and reaches the turning point earlier than the classical particle. But for the backward motion the quantum particle is delayed with respect to the classical particle, resulting in a positive, total time shift. The delay of the quantum particle at the turning-point stems from the finite quantum momentum there and reflects the finite probability for entering the potential barrier. We emphasize, that a negative sign of the total time shift (56) would result in acausal behaviour, because then the quantum particle would leave before it would have arrived, which is not possible. The result (56) allows us to derive a remarkable property of quantum trajectories, that is, they leave the phase-space integral invariant. Comparing the classical and the quantum-mechanical phase-space integrals this can easily be seen. If we define T as the classical period and $2(T_1 + T_2) = T$, we have

$$\oint p(x)\,\mathrm{d}x - ET = \oint \left(p(x) + \operatorname{Re} Q(x)\right)\,\mathrm{d}x - 2E\left\{(T_1 + \Delta t_{\rightarrow}) + (T_2 - \Delta t_{\leftarrow})\right\} \rightarrow$$

$$\oint p(x)\,\mathrm{d}x - ET = \oint p(x)\,\mathrm{d}x - ET + \oint \operatorname{Re} Q(x)\,\mathrm{d}x + 2E\Delta t \Rightarrow$$

$$E\Delta t = -\frac{1}{2} \oint \operatorname{Re} Q(x)\,\mathrm{d}x. \tag{57}$$

From the last line of equation (57) equation (56) readily follows. Thus, if isoenergeticity is fulfilled, the classical and quantum-mechanical motion are described by the same action hypersurface. With the time shift (56), we can now construct the trajectories

$$\begin{aligned}\int_{t_0}^{t_1} \mathrm{d}t' &= \int_{x_{\mathrm{ref}}}^{x} \operatorname{Re} \frac{\partial P(x')}{\partial E}\,\mathrm{d}x' \qquad (x_{\mathrm{ref}} \rightarrow x_2), \\ \int_{t_1+\Delta t}^{t_2} \mathrm{d}t' &= -\int_{x_{\mathrm{ref}}}^{x} \operatorname{Re} \frac{\partial P(x')}{\partial E}\,\mathrm{d}x' \qquad (x_{\mathrm{ref}} \leftarrow x_2).\end{aligned} \tag{58}$$

By this procedure one obtains quantum trajectories in the classically allowed region, forming a sum of disconnected branches

$$x_{\mathrm{q}}(t) = \sum_{n=0}^{\infty}(-1)^n x(t)\theta\left(t_{n+1} - t_n - \Delta t - |t - t_{n+1} + t_n + \Delta t|\right). \tag{59}$$

The trajectories form disconnected branches, because their shape in the classically forbidden region is not available by the trajectory equation (54), but below, when examples will be discussed, we will see how this problem can be solved in a physically reasonable way.

6. Application

To demonstrate how quantum mechanics is done from the Hamilton–Jacobi point of view, we will discuss two important systems that are widely used as models for various physical systems: the linear potential and the harmonic oscillator potential. Especially, we will work out the differences between the Schrödinger point of view and the Hamilton–Jacobi point of view. By this, we will obtain an insight into the quantum-mechanical behaviour, which cannot be gained by the wavefunction alone.

6.1. The linear potential

We consider a linear potential $U(x) = -Fx$. By this example, we will focus on the improvement, that is gained by the use of the zeroth-order quantum correction function $Q_0(x)$ in contrast to the usual WKB approximation. From the potential, we obtain the local classical momentum and the local classical action as

$$p(x) = \sqrt{k^2 + fx}, \tag{60}$$

$$s(x) = \frac{2}{3f}(k^2 + fx)^{3/2}, \tag{61}$$

$$k^2 = \frac{2mE}{\hbar^2}, \qquad f = \frac{2mF}{\hbar^2}. \tag{62}$$

The zeroth-order quantum corrections function in this case can be calculated analytically, giving

$$Q_0(x) = (-\mathrm{i})^{-\frac{1}{3}}\left(\frac{\sqrt{f}}{6}\right)^{\frac{2}{3}}\exp[-\mathrm{i}2s(x)]\Gamma_{1/3}\left[-\mathrm{i}2s(x)\right]. \tag{63}$$

During the following, we set $f = 1$ and $k = 0$, because the system is translationally invariant on the energy axis. In figure 1, we have plotted the phase-space functions of the linear potential. The quantum correction function $\mathrm{Re}\,Q_0(x)$, far away from the classical turning point, here $x_1 = 0$, is negligible and the classical momentum $p(x)$ is in charge. Approaching the turning-point region, the quantum correction function $\mathrm{Re}\,Q_0(x)$ starts to grow, describing the importance of quantum-mechanical behaviour in the vicinity of the turning point. At the turning point itself, the real part of the corrected momentum $\mathrm{Re}\,P(x)$ is finite, while the classical momentum $p(x)$ is zero as usual. This allows only one interpretation: for a classical particle, the potential represents an inpenetrable barrier, and reaching the classical turning point leads undoubtedly to a change of the direction of motion. For a semiclassical particle, described by $\mathrm{Re}\,P(x) = p(x) + \mathrm{Re}\,Q_0(x)$, the classical picture is no longer true. The corrected momentum $\mathrm{Re}\,P(x)$ is finite at the classical turning point, meaning that the potential barrier becomes

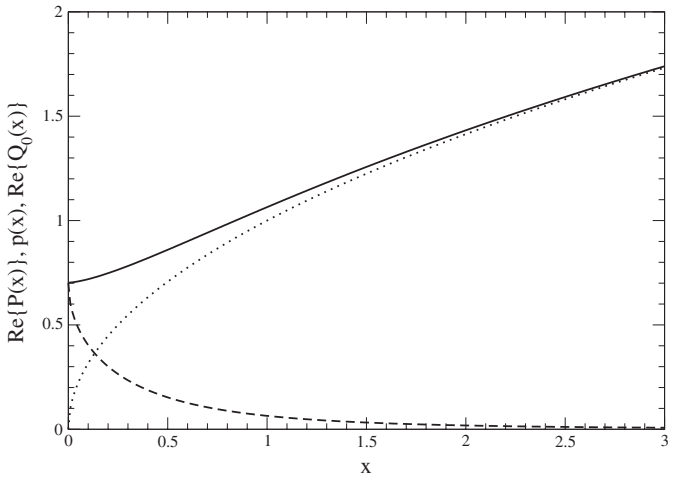

Figure 1. Classically allowed phase space of the linear potential, showing the corrected momentum $\mathrm{Re}P(x) = p(x) + \mathrm{Re}Q_0(x)$ (full line), the quantum correction function $\mathrm{Re}Q_0(x)$ (dashed line) and the classical momentum $p(x)$ (dotted line). The effect of the zeroth-order quantum correction can clearly be distinguished.

penetrable with some probability. For a classical particle, the potential barrier represents a hard wall, but for a semiclassical particle, the potential barrier becomes soft. The softness of the potential barrier in the semiclassical case is described by the finite momentum functions and by the finite probability to find a particle inside the barrier. We want to emphasize here that in the WKB approach the potential barrier remains hard, because of the turning-point singularity. The proper connection between the classically allowed and the classically forbidden regions in the WKB case can only be established by the knowledge of the exact solution of the Schrödinger equation, leading to the reflection phase $\phi = \pi/2$. By the use of quantum correction functions, the turning-point singularity is overcome. The linear potential serves as a model for the one-turning-point case. Taking the turning point x_1 as the turning point of the system, the wavefunction can be constructed by (33):

$$\Psi(x) = \exp\left[-\int_x^\infty \mathrm{Im}Q_0(x')\,\mathrm{d}x'\right]\cos\left[-\int_x^\infty (p(x') + \mathrm{Re}Q_0(x'))\,\mathrm{d}x' - \frac{\phi_{\leftarrow}}{2}\right]. \tag{64}$$

The second turning point x_2 must be set to infinity. This becomes clear when we remember that (33) was derived from the symmetry properties of a two-turning-point system: the particle comes in from infinity until x_1 is reached, where it is reflected back to infinity—and at infinity it is reflected again into the direction of x_1. Thus, a one-turning-point system follows from a two-turning-point system by setting one of the two turning points to infinity. This procedure is necessary, because it is the only way to take into account the symmetry properties of the quantum correction function as discussed above. Together with (39) and the symmetry property of $\mathrm{Im}Q_0(x)$ we obtain the wavefunction

$$\Psi(x) = \exp\left[-\int_{x_1}^x \mathrm{Im}Q_0(x')\,\mathrm{d}x'\right]\cos\left[\int_{x_1}^x (p(x') + \mathrm{Re}Q_0(x'))\,\mathrm{d}x' - \frac{\phi_{\leftarrow}^{\mathrm{inv}}}{2}\right]. \tag{65}$$

Expression (65) perfectly demonstrates how the gauge-dependent part of the reflection phase cancels, while the gauge-invariant part ϕ^{inv} remains present. As can be seen in figure 3 the

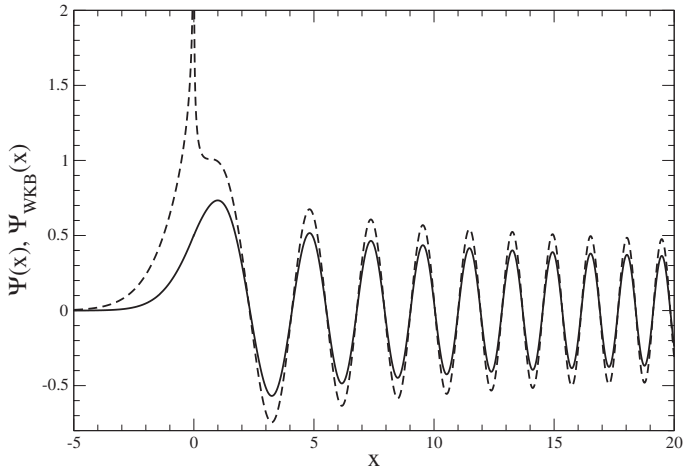

Figure 2. Comparison of the wavefunction obtained by the zeroth-order quantum correction function (full line) and the usual WKB approximation (dashed line). Already the zeroth-order quantum correction removes the WKB-turning-point singularity completely and is, up to the amplitude, identical with the exact solution of the corresponding Schrödinger equation, the Airy function.

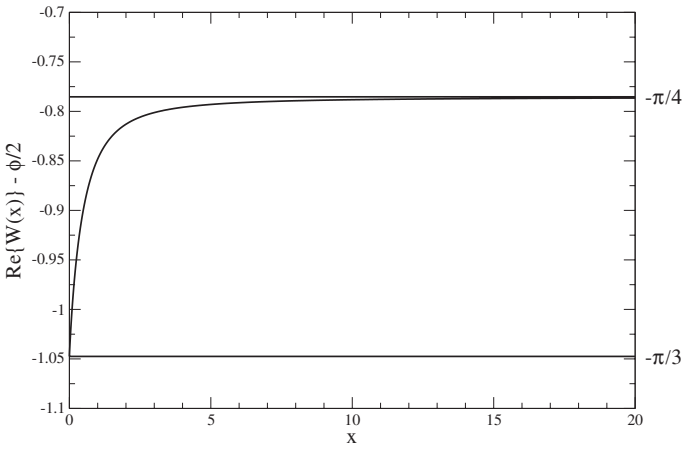

Figure 3. Illustration of how the correct asymptotic reflection phase is approached by the interplay of the real part of the quantum action correction and the kinematical phase.

invariant phase $\phi^{\mathrm{inv}} = 2\pi/3$ is not the WKB reflection phase $\pi/2$ obtained by the asymptotical expansion of the Airy function. The asymptotical reflection phase follows from the limit

$$\lim_{x\to\infty}\int_{x_1}^{x} \mathrm{Re}\,Q_0(x')\,\mathrm{d}x' - \frac{\phi_{\leftarrow}^{\mathrm{inv}}}{2} = -\frac{\pi}{4}. \tag{66}$$

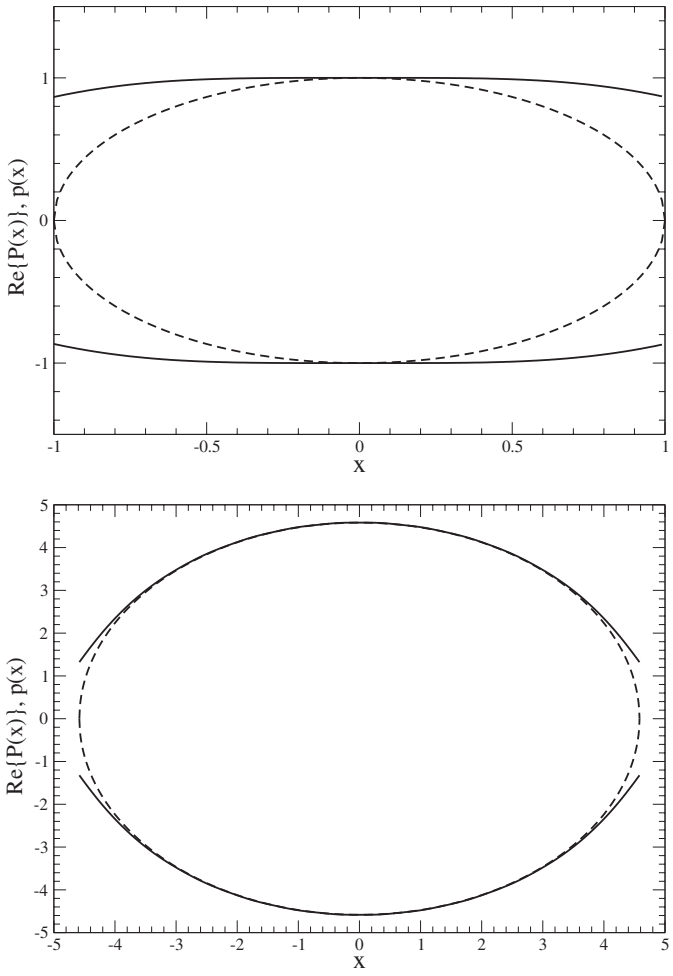

Figure 4. Comparison of the phase space of the harmonic oscillator for the full quantum momentum $\mathrm{Re}P(x) = p(x) + \mathrm{Re}Q(x)$ (full line) and the classical momentum $p(x)$ for the ground state (above) and the tenth excited state (below). Due to the soft boundary conditions, the quantum-mechanical phase space is an open ellipse, while the classical phase space is the well-known closed ellipse.

6.2. The harmonic oscillator

The harmonic oscillator is surely the most considered and best understood quantum system. This fact makes it a very interesting test object for the viewpoint on quantum mechanics that we haves developed here, because by the harmonic oscillator, we can demonstrate at best the differences between the Schrödinger and Hamilton–Jacobi quantum mechanics.

We will work in suitably scaled quantities

$$p(x) = \sqrt{k^2 - \Omega^2 x^2}, \qquad k = \sqrt{\frac{2mE}{\hbar^2}}, \qquad \Omega = \frac{m\omega}{\hbar}. \tag{67}$$

For simplicity, but without loss of generality, we have set $\Omega = 1$ in all numerical calculations. In figure 4, we have plotted the quantum-mechanical and the classical phase space of the harmonic oscillator for the ground-state energy (top picture). Again we see the typical effect

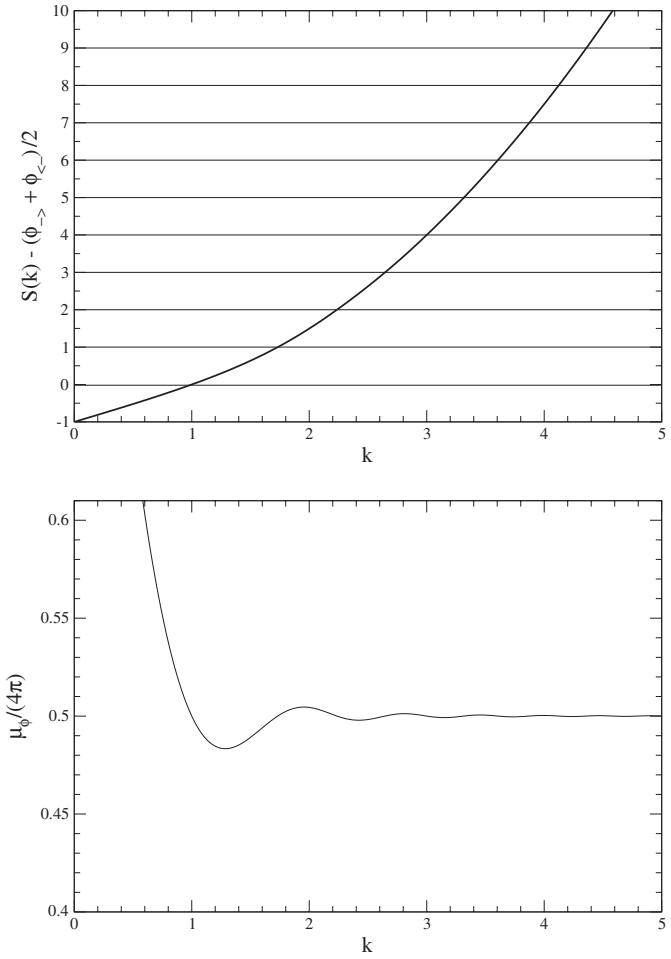

Figure 5. Quantization curve and $\mu_\phi/(4\pi)$ for the harmonic oscillator in units of π.

of the quantum correction functions, breaking up the closed classical phase space, thus making the potential barrier soft and penetrable. The effect of the quantum correction functions is largest for the ground state, as one would naturally expect, because the ground state is close to the anticlassical limit of the system. For the tenth excited state, the bottom picture in (4) shows that the influence of $Q(x)$ already has declined, the system has already entered its semiclassical limit and quantum corrections become negligible.

We will not present the pictures of oscillator wavefunctions here, because we think that up to now the reader might be convinced that the wavefunctions determined by (30) or (33) are, up to the normalization amplitude, identical with the oscillator wavefunctions determined by the Schrödinger equation. Instead we will focus on the calculation of quantities that are not available within the Schrödinger equation. In figure 5, we have calculated the quantization curve and the Maslov index according to formulae (40) and (41). The quantization curve determines the oscillator eigenstates by knowledge of the classical momentum and its quantum corrections. Although the wavefunction is implicitly known when the reflection

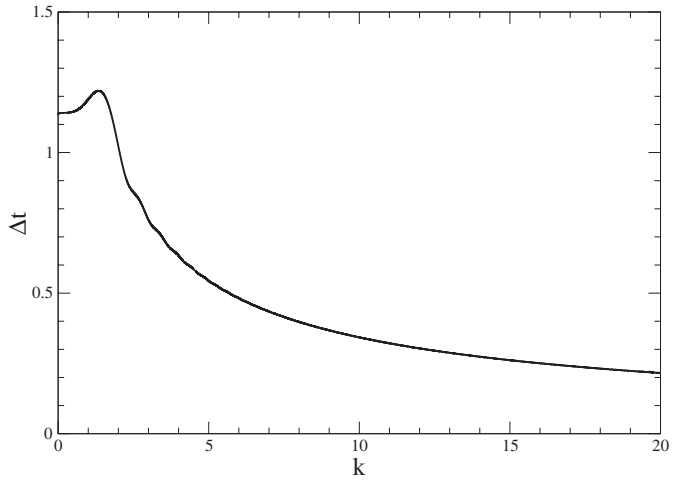

Figure 6. Total time shift Δt as a function of k. For high energies, the total time shift tends to zero, because the system approaches its classical limit, where quantum and classical trajectories do no longer differ.

phases (38) and (39) are known, there is no need to employ them for determining the spectrum. The knowledge of the quantum correction functions is sufficient for a calculation from first principles. The Maslov index imposes a tiny oscillating structure onto the quantization curve. The nodes of these oscillations lie perfectly at $1/2$, coincidence with the bound states and recover the Bohr–Sommerfeld rule. This behaviour of the Maslov index was first calculated in [15] for the half-sided harmonic oscillator and by a different method.

6.3. Trajectories for the harmonic oscillator

For the harmonic oscillator, we now will discuss the topic of quantum trajectories in detail. We will calculate and discuss trajectories for the ground state and the tenth excited state to illustrate the influence of the quantum correction functions near the anticlassical and in the semiclassical regime.

By (56) the time shift between the quantum and classical motion, see figure 6, is given as

$$\Delta t = -\frac{2}{k}\int_0^{x_2} \frac{\partial\, \mathrm{Re}\, Q(x)}{\partial k}\,\mathrm{d}x. \tag{68}$$

The lower bound in (68) is zero, because we want to calculate the trajectory of a particle starting its journey from the minimum of the oscillator potential $x = 0$. We could have chosen any other point, the choice of the point of reference has no influence on the shape of the quantum trajectory. From the trajectory equation (54), we get

$$x_{\mathrm{q}}(t) = \sum_{n=0}^{\infty}(-1)^n x(t)\theta(t_{n+1} - t_n - \Delta t - |t - t_{n+1} + t_n + \Delta t|), \tag{69}$$

where the index n denotes the multiple branches obtained by shifting the time by Δt in the classically allowed region for the forward and backward motion. By the trajectory equation (54) only the quantum motion between the two turning points can be determined.

The cutoff at the turning points is the cause the multiple branches. If we compare (69) with the classical trajectory

$$x_{\mathrm{cl}}(t) = \sqrt{\frac{k^2}{\Omega^2}}\sin[\Omega t], \tag{70}$$

and use the fact that quantum and classical motion are described by the same frequency, see (57), we are led to make the following ansatz for a quantum trajectory

$$x_{\mathrm{q}}(t) = A_{\mathrm{q}}(k, \Omega, t)\sin[\Omega t], \qquad \lim_{k\to\infty} A_{\mathrm{q}}(k, \Omega, t) = \sqrt{\frac{k^2}{\Omega^2}}. \tag{71}$$

The limit in (71) requires, that the quantum amplitude approaches its classical value in the classical limit. The fact that all quantum effects are now located in an amplitude function reminds us of the path integral, where the same phenomenon occurs: phase quantities are given by the classical action function, but the time-evolution amplitude is quantum mechanical. However, by comparison between (69) and (71), we can establish a continuous quantum trajectory without cutoffs at classical turning points by analytical continuation beyond the classical turning points, illustrated in figure 7. The reader might object this procedure by the argument that by analytical continuation in this case a kind of information is gained, which does not exist. We agree with this argument to some extent and will therefore call the trajectories in the classically forbidden region apparent trajectories. The present situation is similar to the quantum time shifts in [18], where it was found that the apparent trajectories enter the classically forbidden region. But the difference between there to present is that in [18] the potential was a singular one—and no particle, classical or quantum can cross a singularity. But the harmonic oscillator is regular and by the quantum correction functions, the turning-point region has become regular, too. Further we know from above that in the quantum case the potential becomes soft and therefore penetrable. All this put together means the following: for the harmonic oscillator, the reflection probability at a turning point is $|R(k_n)|^2 = 1$ for all energies, thus the particle comes back in any case. The particle reaches the classical turning point with finite momentum, which imposes a time shift in comparison to the classical particle and a phase shift on the wavefunction as a result of the soft boundary condition to be fulfilled. The phase shift of the wavefunction and the time shift of the motion are two manifestations of the same phenomenon; the relative softness of the potential barrier in the quantum-mechanical limit. All these facts allow only one interpretation, the particle as it has arrived at the turning point with finite momentum, goes beyond the turning point and enters the classically forbidden region, appears to be decelerated by the soft barrier, comes to rest and finally moves backwards to be expelled again into the classically allowed region. The only explanation thus is the softness effect of the potential barrier. We emphasize, that this softness has nothing to do with sticking or absorptive reactions; it is a pure quantum-mechanical effect. For energies approaching the classical limit, the barrier hardens as is described by the limiting process in (71).

7. Summary and conclusion

We have shown how quantum-mechanical problems can be solved within the framework of the Hamilton–Jacobi equation of quantum mechanics, where the central quantity of interest is the quantum-mechanical action function instead of the wavefunction. To our regards, the Hamilton–Jacobi theory and Schrödinger theory are fully equivalent to each other; they describe the same physics and differ only in their descriptive manner.

In contrast to the well-known Madelung–de Broglie–Bohm theory, we do not separate the real and imaginary parts of the action function initially. A very valuable feature of the

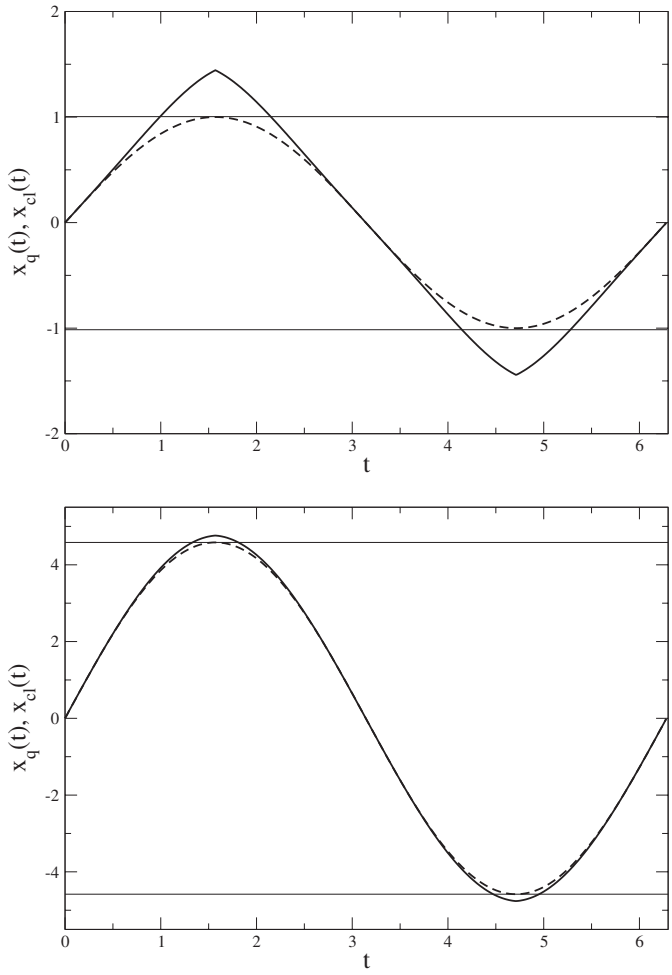

Figure 7. Comparison of quantum trajectories (full lines) and classical trajectories (dashed lines). The full lines are the branches obtained by the trajectory equation (54). The total time shift Δt is the amount of time the quantum particle spends in the turning-point region. It can be clearly seen, how the limiting process from (71) works.

Hamilton–Jacobi theory is, that by the use of the quantum action function, the wavefunction can uniquely be decomposed into running waves at every point in space, regardless of whether the wavefunctions describe bound or scattering states. In the Schrödinger point of view, this is possible only asymptotically.

The use of quantum correction functions opens a deeper insight into the quantum-mechanical behaviour of systems, especially in the vicinity of turning points, where the local quantum-mechanical momentum is finite. This property overcomes the WKB singularity at classical turning points and furthermore clarifies the special behaviour of a potential barrier in the quantum-mechanical case: the barrier becomes soft and therefore allows the quantum particle to enter it. This softness property of the potential barrier in the quantum-mechanical case is modelled by the soft boundary conditions the wavefunction has to obey—and that can be solved exactly by help of the quantum action function—and also explain the finite probability of finding a particle there.

The soft boundary-value problem is solved by a reflection phase. The reflection phase is the key quantity to obtain the spectrum of a quantum system with the help of a quantization curve and allows a direct calculation of Maslov indices. To obtain the spectrum of a quantum system by this method, only action and momentum functions have to be known, orthonormalized wavefunctions are not necessary. Especially for potentials where exact wavefunctions are not analytically known, it may be much more simple to calculate the quantization curve instead of searching orthonormalized eigenstates with the Schrödinger equation.

Besides, the Hamilton–Jacobi theory allows us to calculate quantities that are not available within the Schrödinger point of view; the calculation of quantum trajectories is possible. The quantum trajectories obtained by the trajectory equation (54) are only defined in the classically allowed region, but by analytical continuation, they can also be established for the classically forbidden region in a physically reasonable manner. The behaviour of the trajectories again mirrors the softness-property of the potential barrier in the quantum-mechanical case and the finite probability to enter the classically forbidden region is all described by a total time shift Δt (56). In contrast to de Broglie–Bohm theories, no quantum potential is introduced, and therefore no equation of motion. Moreover, the equation of motion in de Broglie–Bohm theories [3–5] and our trajectory equation (54) contradict each other. This result was also found by [7, 8], but was interpreted differently. Although the trajectories obtained from the quantum action integral by the use of the Hamilton–Jacobi formalism show a somewhat quirky behaviour, they are consistent with our results about the behaviour of the quantum correction function in the vicinity of classical turning points and the behaviour of the wavefunction. Both, quantum correction functions and trajectories illustrate the softness of a potential function near the anticlassical limit. Moreover, the Hamilton–Jacobi formalism is theoretically very well founded and thus we expect ourselves to travel on safe terrain, whereas, as stated in [16, 17] the equivalence between velocity and quantum-mechanical momentum in de Broglie–Bohm theories is up to now an unproved assumption.

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