Wentzel-Kramers-Brillouin method in the Bargmann representation

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We demonstrate that the Bargmann representation of quantum mechanics is ideally suited for semiclassical analysis, using as an example the WKB method applied to the bound-state problem in a single well of one degree of freedom. While the WKB expansion formulas are basically the usual ones, in this representation they describe approximations that are uniform and nonsingular in the classically allowed region of phase space because no turning points appear there. The quantization of energy levels relies on a complex contour integral that tests the eigenfunction for analyticity. For the harmonic oscillator, this WKB method trivially gives the exact eigenfunctions in addition to the exact eigenvalues. For an anharmonic well, a self-consistent variational choice of the representation greatly improves the accuracy of the semiclassical ground state. Also, a simple change of scale illuminates the relationship of semiclassical versus linear perturbative expansions, allowing a variety of multidimensional extensions. All in all, the Bargmann representation appears to combine the advantages of a linear description and of a phase-space representation of the quantum state vectors.

INTRODUCTION

The purpose of this paper is to provide a self-contained presentation of certain results and formulas selected from one of our previous unpublished works.[1] This will be a selection of these results which pertain to the usefulness of combining WKB techniques with Bargmann's representation of quantum mechanics. While we are adding here no basically new result to Ref. 1, we have streamlined the presentation and included more recent references on related topics.

A recurrent problem in semiclassical analysis is the construction of global uniform approximations to the wave functions. This difficulty is fully present in bound states, where it is the major obstacle in the derivation of quantization formulas for the discrete energy levels. While WKB wave forms are very simple and powerful approximations, they fail at the caustics and require extra matching procedures to be developed. Phase-space methods in quantum mechanics eliminate the caustic singularities on physical grounds, but they are "bilinear" in the wave functions; the local phases of the wave functions are very hard to recover, and energy quantization crucially depends on this type of information.

Bargmann[2] has introduced a representation of quantum mechanics where a creation operator, typically $(\hat{q}-i\hat{p})/\sqrt{2}$, is diagonalized. In this representation, wave functions are holomorphic (entire) functions of the complex variable $z=(q-ip)/\sqrt{2}$. If we write and solve the Schrödinger equation directly in this representation, we combine the advantages of a *linear* method (presence of a wave equation, explicit phase information in the wave function), and the benefits of a *phase-space method* (inasmuch as the complex z variable acts as a phase-space coordinate). The genuine difficulties in the physical interpretation of the Bargmann theory are irrelevant here: we only use this representation as a computational device. The purpose of this article is to describe various advantages of doing WKB analysis directly in Bargmann space. The WKB solutions are automatically global and uniform over connected trajectories; no matching is required. The Bohr-Sommerfeld loop integral for energy quantization can be explained in terms of analytic function theory. The transition toward low quantum numbers and down to the ground state can be more neatly described, allowing for an actual numerical improvement of the method in that region of the spectrum.

While the interest of the Bargmann representation for semiclassical analysis has been recognized elsewhere, it was with emphasis on time-evolution problems and especially on the Feynman path integral.[3]

I. GENERALITIES AND NOTATIONS

We shall confine our interest to the *bound-state* problem for the Schrödinger equation in one degree of freedom (the real line),

$$H\psi=E\psi\ . \tag{1.1}$$

(However, scattering or time-dependent problems could also benefit from the methods to be described.)

We recall first some general facts about the semiclassical analysis of such a problem, giving the notations at the same time. Two successive stages are involved: the *equation* must have a classical analog in the limit $\hbar\to 0$, and the implied restrictions on the observable H must be stated; *solutions* can then be sought as functions of the parameter $\hbar$ becoming asymptotically correct as $\hbar\to 0$.

A. Semiclassical observables

The first question is often answered implicitly by specializing the Hamiltonian, e.g., $H=-\hbar^2\Delta+V(q)$. Howev-

er, we shall need later broad canonical invariance properties. (Moreover, in view of higher-dimensional extensions, additional constants of the motion must be taken into account, which do not have this form.) For these reasons we prefer a formalism which allows the Hamiltonian to be a rather general observable.

In classical mechanics an observable like the Hamiltonian is a smooth function $h(q,p)$ on phase space (the plane). A quantization map associates to $h(q,p)$ an operator function $H=h(\hat{q},\hat{p})$ subject to a particular ordering rule of the operator arguments $\hat{q}$ and $\hat{p}$ (which are the standard ones, obeying $[\hat{q},\hat{p}]=i\hbar$). The inverse transformation maps H to a classical function h, which is then called the symbol of the operator H, $h=H_S$. The central idea in semiclassical analysis is to manipulate quantum operators entirely through their symbols. The basic requirements are thus (1) that the quantization map should be linear, and invertible (on suitable subspaces) so that the inverse symbol map be well defined, and (2) that attention should be restricted to these quantum observables H which have an admissible behavior in the semiclassical limit, e.g.,

$$H_S(\hbar;\mathbf{x}) \underset{\hbar\to 0}{\sim} \sum_{n=0}^{\infty} \hbar^n H_n(\mathbf{x}) , \tag{1.2}$$

where expansion coefficients $H_n(\mathbf{x})$ are smooth functions of the point $\mathbf{x}=(q,p)$ in phase space. The leading term $H_0(\mathbf{x})$ gives the classical limit (as an observable) of H; the remaining terms allow for quantum corrections of any order in $\hbar$ to be present.

Two quantization orderings will be especially convenient for us: Weyl (symmetric), and Wick (normal) ordering. The inverse maps respectively associate with an operator H the Weyl symbol H_W (Refs. 4–6 and 1) and the normal symbol H_N.[7,1] The Weyl symbol is

$$H_W(\hbar;q,p)=\int_{-\infty}^{\infty} \langle q-r/2|H(\hbar)|q+r/2\rangle e^{ipr/\hbar} dr , \tag{1.3}$$

and it is covariant under translations and linear canonical transformations of phase space.

The normal symbol, by contrast, depends on the choice of a reference harmonic oscillator, or equivalently of a complex coordinate z to represent the two-dimensional phase space. In suitable coordinates, we have

$$z=(q-ip)/\sqrt{2}, \quad z^*=(q+ip)/\sqrt{2} , \tag{1.4}$$

giving the reference harmonic oscillator as

$$h(q,p)=z^*z=\tfrac{1}{2}(q^2+p^2)=\tfrac{1}{2}\|x\|^2 . \tag{1.5}$$

Here, however, we have sacrificed the full linear canonical invariance, keeping only rotational (and always translational) invariance. This sacrifice will be in fact profitable for certain purposes, see Sec. IV B.

The normal symbol of the operator H is then the expectation value

$$H_N(\hbar;q,p)=\langle \Omega_{q,p}|H|\Omega_{q,p}\rangle , \tag{1.6}$$

where $|\Omega_{0,0}\rangle$ is the normalized ground state of the reference harmonic oscillator (1.5) quantized and $|\Omega_{q,p}\rangle$ is obtained by displacing $|\Omega_{0,0}\rangle$ to the phase-space location (q,p) according to

$$|\Omega_{q,p}\rangle=\exp\frac{i}{\hbar}(p\hat{q}-q\hat{p})|\Omega_{0,0}\rangle . \tag{1.7}$$

The inverse quantization, or mapping from the function $H_N(q,p)$ to the operator H, is simply normal ordering with respect to the operators $\hat{z}$ and $(z^*)\hat{}=\hat{z}^\dagger$, which are, respectively, the quantum creation and destruction operators for the harmonic oscillator $\hat{h}$. If the normal symbol is expressed in terms of the complex coordinates,

$$H_N(z,z^*)=H_N\left[q=\frac{z+z^*}{\sqrt{2}}, p=\frac{z^*-z}{i\sqrt{2}}\right] , \tag{1.8}$$

then the quantum operator is

$$H=H_N(\hat{z},\hat{z}^\dagger) \tag{1.9}$$

with $\hat{z}^\dagger$ operators systematically ordered to the right of all $\hat{z}$ operators.

For a given quantum operator H, its normal symbol can also be obtained by a Gaussian smearing in phase space of its Weyl symbol

$$H_N(\hbar,\mathbf{x})=\int H_W(\hbar;\mathbf{x}')(\pi\hbar)^{-1}e^{-\|\mathbf{x}-\mathbf{x}'\|^2/\hbar}dx' . \tag{1.10}$$

This operation can also be expanded order by order in $\hbar$, giving

$$H_N(\hbar;\mathbf{x})\sim\exp\left[\frac{\hbar}{4}\left[\frac{d^2}{dq^2}+\frac{d^2}{dp^2}\right]\right]H_W(\hbar;\mathbf{x}) . \tag{1.11}$$

B. Semiclassical states

The next question is that of understanding how the solutions of Eq. (1.1) (the eigenfunctions and eigenvalues) reflect the limiting classical dynamics in their dependence on the parameter $\hbar$ when $\hbar\to 0$: we want to describe the quantum eigenstates semiclassically.

To study a quantum state vector $|\psi\rangle$, we may apply a symbol map to the projector onto it, $|\psi\rangle\langle\psi|$. The resulting Weyl symbol $(|\psi\rangle\langle\psi|)_W$ is also called the Wigner function of the state,[8] and the normal symbol,

$$(|\psi\rangle\langle\psi|)_N(\hbar;q,p)=|\langle\Omega_{q,p}|\psi\rangle|^2 , \tag{1.12}$$

is also called the Husimi function.[9] Either of them provides a convenient phase-space representation of the quantum state, endowed with a nice semiclassical behavior: as $\hbar\to 0$, they must tend to a classical phase-space distribution, which can even be sometimes determined. In general, however (i.e., in more than one degree of freedom), this information is not sufficient to reconstruct the wave function itself. The quantum phase, which controls the fast oscillations of the symbol, is obliterated in the limiting process and cannot be regenerated easily. Hence the fine details of eigenstates and of the eigenvalue spectrum are often not known in any explicit form (case of classically chaotic systems). Some more regular cases will admit some semiclassical wave functions, but the explicit forms of these depend on idiosyncrasies of the clas-

sical dynamics; and they are by no means universal. It is only for one degree of freedom (and, by extension, for completely integrable systems) that a full theory of semiclassical wave functions is available, based on WKB (also called phase-integral) approximations.

It is so difficult to reconstruct the full wave vector ψ from the semiclassical form of the Wigner (or Husimi) function perhaps because this function depends bilinearly on ψ.

II. THE BARGMANN REPRESENTATION (REF. 2)

The complex phase-space variables $z=(q-ip)/\sqrt{2}$, $z^*=(q+ip)/\sqrt{2}$ are also canonically conjugate to each other (up to a factor i). This holds both classically,

$$\{z,z^*\}=i \quad (\{q,p\}=1) \tag{2.1}$$

and quantum mechanically,

$$[\hat{z},\hat{z}^\dagger]=-\hbar \quad ([\hat{q},\hat{p}]=i\hbar) . \tag{2.2}$$

Now, the Schrödinger representation of quantum states diagonalizes the position operator $\hat{q}$, expressing pure states as wave functions $\psi(q)$, with $\hat{p}=-i\hbar d/dq$. Likewise, the Bargmann representation diagonalizes the creation operator $\hat{z}$ and expresses states as functions $\psi(z)$, the basic operators being (in one degree of freedom)

$$\begin{aligned} &\hat{z} \text{ (denotes multiplication by } z) , \\ &\hat{z}^\dagger=\hbar d/dz . \end{aligned} \tag{2.3}$$

The transformation $\psi(q)\overset{B}{\rightarrow}\psi(z)$ is given by

$$\psi(z)=(\pi\hbar)^{-1/4} \times \int_{-\infty}^{\infty} \exp\left[\frac{1}{\hbar}\left[-\frac{q^2+z^2}{2}+\sqrt{2}zq\right]\right]\psi(q)dq . \tag{2.4}$$

This maps the standard Hilbert space $L^2(dq)$ over the Hilbert space of entire (analytic) functions $\psi(z)$ with finite norm, this norm being

$$\langle\psi(z)|\psi(z)\rangle=(2\pi\hbar)^{-1}\int[\psi(z)]^*\psi(z)e^{-|z|^2/\hbar}dq\,dp . \tag{2.5}$$

We also have the relation

$$\psi(z)=e^{|z|^2/2\hbar}\langle\Omega_{q,p}|\psi\rangle , \tag{2.6}$$

which exhibits the connection between the Bargmann representation and the various coherent-state approaches to quantum mechanics.[10] Compared with the Husimi function (1.12), $\psi(z)$ carries phase information explicitly.

Both the differences and the similarities between the Bargmann representation and others make it an extremely attractive tool for semiclassical analysis.[1] The Bargmann representation diagonalizes the operator $\hat{z}$, whose complex eigenvalue can be viewed as a phase-space variable, $z=(1/\sqrt{2})(q-ip)$. Its global and analytical structure are quite different from the Schrödinger picture, reflecting the fact that $\hat{z}$ is a combination of two observables which cannot be simultaneously measured in quantum mechanics. Nevertheless, the function $\psi(z)$ can be conceived as a sort of phase-space representation of the quantum state $|\psi\rangle$. Phase-space representations are very useful in semiclassical theory because classical trajectories have no caustics in phase space (thanks to Liouville's theorem). However, the Wigner (or Kirkwood, Husimi, etc.) functions which are traditionally used for this purpose are bilinear in the wave function, which is in a way natural but also creates some big technical difficulties.

Now, the Bargmann representation is similar to the Schrödinger representation in that it is linear in the wave function, and that moreover all formulas of an algebraic nature can be taken over from the better-known Schrödinger picture because the algebras are essentially isomorphic. This is especially true for all semiclassical expansion coefficients, which are algebraic functions of the symbols and their derivatives.

In other words, the semiclassical expansion algorithms are the same. We simply must now apply them directly to the Schrödinger equation written in the Bargmann representation, i.e.,

$$H\left[z,\hbar\frac{d}{dz}\right]\psi(z)=E\psi(z) . \tag{2.7}$$

The exact operator meaning of $H(z,\hbar d/dz)$ is, for instance, the normal-ordered quantization of the normal symbol $H_N(z,z^*)$, as in Eq. (1.9). Symbols may, in full generality, contain $\hbar$-dependent "quantum corrections." For instance, the standard harmonic oscillator $\hat{h}=(\hat{p}^2+\hat{q}^2)/2$ has the normal symbol $h_N=z^*z+\hbar/2$ and in the Bargmann representation its normal-ordered quantization is

$$\hat{h}=\hbar z\frac{d}{dz}+\hbar/2 . \tag{2.8}$$

But we could have started instead with the Weyl symbol $h_W=z^*z$, which upon Weyl ordering gives

$$\hat{h}=\frac{1}{2}\left[z\left[\hbar\frac{d}{dz}\right]+\left[\hbar\frac{d}{dz}\right]z\right] , \tag{2.9}$$

the same operator as Eq. (2.8).

Either symbol representation of the given quantum Hamiltonian H has its own advantages as a basis for the semiclassical expansion of the eigenfunction. The corresponding algorithms differ by small algebraic details and will be described in turn.

III. THE WEYL-WKB-BARGMANN METHOD IN ONE DEGREE OF FREEDOM

It is well known in the usual representations of quantum mechanics that the WKB method provides the most powerful analytical semiclassical description for eigenfunctions in one degree of freedom. . . if it were not for the turning points (or caustics). The method can only be made global and uniform, then, at the expense of complicated constructions (using either special functions, or complex paths, or the patching of various local represen-

tations). Very useful eigenvalue formulas are then obtained [Bohr-Sommerfeld, Maslov, or Einstein-Brillouin-Keller (EBK) rules].

We shall now transcribe the WKB method to the Bargmann representation and show that it immediately gives singularity-free, global approximations in the useful region, for a single well potential. No matching is needed, nor any shuttling back and forth between representations. Quantization rules, relations with perturbation theory become transparent and exhibit strong connections with analytic function theory.[1]

In this section we discuss the formulas attached to the use of the Weyl symbol for the Hamiltonian, whereas the normal symbol will be used in Sec. IV.

A. The WKB wave construction

We want to construct a WKB, or phase-integral, solution to $H\psi=E\psi$ in the Bargmann representation based on the Weyl symbol $H_W(\hbar;x)$. We shall develop the calculation to leading order in $\hbar$ (dominant semiclassical behavior). We moreover assume that H_W does not depend on $\hbar$, i.e., that it coincides with the classical Hamiltonian. It is in fact surprisingly simple to incorporate quantum corrections to all orders if the appropriate algorithm is used; this is done in Appendix A. (The corrections only involve *even* powers of $\hbar$ in the Weyl formalism.)

We know that in the Schrödinger representation, the equation $H\psi=E\psi$ admits local asymptotic solutions

$$\psi(q)\underset{\hbar\to 0}{\sim}\left[\frac{\partial H_W}{\partial p_E}\right]^{-1/2}\exp\left[\frac{i}{\hbar}\int^q p_E(q')dq'\right] \tag{3.1}$$

where $p_E=p_E(q)$ is any branch of the classical energy curve in phase space,

$$H_W(q,p)=E\ . \tag{3.2}$$

That Eq. (3.1) satisfies the Schrödinger equation up to $O(\hbar^2)$ results from a purely algebraic computation. Since Weyl ordering looks the same in the Schrödinger and Bargmann representations (this involves the invariance under a linear, albeit complex, canonical transformation), the same formulas apply *mutatis mutandis* in the Bargmann representation. We must simply replace (q,p) by (z,z^*) and $\hbar$ by $i\hbar$, to find that the eigenvalue equation admits local asymptotic solutions

$$\psi(z)\sim\left[\frac{\partial H_W}{\partial z_E^*}\right]^{-1/2}\exp\left[\frac{1}{\hbar}\int^z z_E^*(z')dz'\right]\ , \tag{3.3}$$

where $z_E^*(z)$ is a branch of the classical energy curve in the (z,z^*) coordinates

$$H_W(z,z^*)=E\ . \tag{3.4}$$

Equation (3.3) can also be derived by applying the integral transformation (2.4) to the coordinate space WKB solution (3.1), using the complex stationary phase method to perform the integration. The integral $\int^z z_E^*(z')dz'$ simply gives the classical action in the z variable.

Now, the relation $H_W(z,z^*)=E$ and the fact that z^* is the complex conjugate of z imply that z lies over the real energy curve, i.e., $z=[q-ip_E(q)]/\sqrt{2}$ for some q, and consequently $z_E^*(z)=[q+ip_E(q)]/\sqrt{2}$. This defines a preferred branch $z_E^*(z)$ of the curve (3.4) over the real classical energy curve only, but this branch is single valued by construction. For nonanalytic H_W it may happen that it is impossible to extend the function $z_E^*(z)$ anywhere outside. Thus the asymptotic expression (3.3) is well defined in any case only for z *over* the real energy curve.

There, however, the WKB expression (3.3) has no turning point anywhere, hence it is globally regular. Indeed, the turning point condition,

$$\frac{\partial H_W}{\partial z^*}=0\ , \tag{3.5}$$

and reality, imply $\partial H_W/\partial z=0$ as well. Then it is the phase-space velocity on the classical orbit which must vanish, but this only takes place for singular orbits which are stationary points of $H_W(q,p)$, and which are anyway excluded from the scope of the WKB method (see, however, Sec. IV C).

B. Semiclassical eigenvalues

Energy quantization around a closed energy curve is now immediate: the global approximation (3.3) must be single valued over the energy curve, implying

$$\oint z_E^*(z)dz=2\pi i\hbar\left[k+\frac{\alpha}{2}\right]\ , \tag{3.6}$$

where α is the winding number of the function $\partial H/\partial z_E^*$ around one turn. On the left-hand side, by canonical invariance,

$$\oint z_E^*(z)dz=i\oint p_E(q)dq\ , \tag{3.7}$$

so that we recover the standard EBK eigenvalues provided we identify α with the Maslov correction.

Another interpretation of the quantization rule (3.6) is that it monitors whether the eigenfunction $\psi(z)$ is analytic inside the real energy contour. A necessary condition for analyticity is

$$\frac{1}{2\pi i}\oint\frac{\psi'(z)}{\psi(x)}dz=k'\ , \tag{3.8}$$

which must be a *non-negative* integer, giving the number of zeros of $\psi(z)$ (counted with their multiplicities) which lie inside the energy curve. If we use the approximation (3.3) on the energy contour, we find exactly the condition (3.6), and moreover $k'=k$: the kth eigenfunction has precisely k zeros inside the energy curve (cf. Sturm-Liouville theory).

There is a marked difference here with quantization in the Schrödinger representation: the eigenvalue selection is effectively achieved here by enforcing not the square integrability of the eigenfunction (i.e., restricting its growth at infinity), but is analyticity (which is the other condition for belonging to the Bargmann vector space).

C. Analytical extension (Ref. 1)

Since analyticity in z is an important feature in the Bargmann theory, it is natural to consider in more detail

the frequent case where the classical Hamiltonian $H_W(z,z^*)$ itself is analytic in both variables z and z^*. The energy relation $H_W(z,z^*)=E$ then implicitly defines z_E^* as a multiply valued (i.e., ramified) analytic function of the complex variable z. Outside the real energy curve, $z_E^*(z)$ is no longer the complex conjugate of z, so that a less confusing notation is required. We shall denote as y the independent complex variable canonically conjugate to z (in the sense of classical mechanics), i.e.,

$$z=(q-ip)/\sqrt{2},\quad y=(q+ip)/\sqrt{2}$$

(q,p now complex) . (3.9)

The complex energy curve is then defined by

$$H_W(z,y)=E\ , \tag{3.10}$$

its explicit branches are locally analytic functions of z,

$$y=y_E(z)\ , \tag{3.11}$$

which connect (generally two by two) at the complex turning points, given by

$$\frac{\partial H_W}{\partial y_E}=0\ . \tag{3.12}$$

There remains a privileged branch $y_E^{(0)}(z)$ such that the real energy curve is specified by $y_E^{(0)}(z)=z^*$, and for regular energy values this real curve contains no turning point, as explained before. We can think of the cut plane carrying the branch $y_E^{(0)}(z)$ as the principal or first sheet of the function $y_E(z)$.

The WKB approximation itself is now a holomorphic expression of z in a region about the real energy curve avoiding turning points in the first sheet:

$$\psi(z)\sim\left[\frac{\partial H_W}{\partial y_E^{(0)}}\right]^{-1/2}\exp\left[\frac{1}{\hbar}\int^z y_E^{(0)}(z')dz'\right]\ . \tag{3.13}$$

However, the true eigenfunction $\psi(z)$ is certainly approximated by this simple expression only in some annular neighborhood of the real energy curve (Fig. 1). Further away, other branches $y_E(z)$ could contribute as well, so that a global approximation of $\psi(z)$ in the whole z plane would still involve computations of connection formulas, Stokes phenomena, etc. The crucial advantage of the Bargmann representation is that this extra work is only required if subdominant (i.e., exponentially small) quantities are wanted. Within asymptotic accuracy, everything is controlled by the values of $\psi(z)$ over a vicinity of the real classical orbit in the principal sheet.

Analyticity also makes eigenvalue calculations more flexible. The complex integration contour in Eq. (3.5) may be deformed from its initial position over the real orbit, as long as it stays away from turning points and cuts of the ramified holomorphic function $y_E^{(0)}(z)$.

Consequently, if we interpret Eq. (3.6) as counting the number of zeros of the exact eigenfunction $\psi(z)$, we find that these zeros must accumulate in the classical limit along certain cuts joining pairs of turning points (these cuts must be anti-Stokes lines).

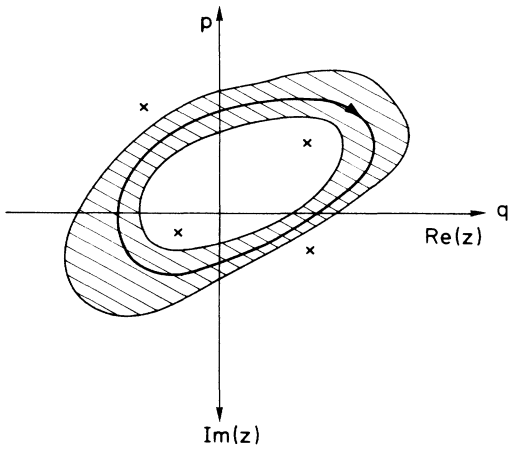

FIG. 1. Typical configuration of a real classical orbit and of complex turning points in the Bargmann representation. The dashed area suggests the region of uniform validity for the WKB approximation.

D. The harmonic oscillator (Refs. 11 and 1)

In the Bargmann representation, the Hamiltonian for the reference harmonic oscillator, Eqs. (2.8)–(2.9), is of first order d/dz, and this causes the leading WKB approximation to become trivially exact for the eigenfunctions (and thereby for the eigenvalues). Specifically, we have the equation

$$\left[\hbar z\frac{d}{dz}+\frac{\hbar}{2}\right]\psi(z)=E\psi(z)\ . \tag{3.14}$$

The Weyl symbol being $H_W(z,y)=yz$, the WKB formula (3.13) gives

$$\psi(z)=z^{-1/2}\exp\left[\frac{1}{\hbar}\int^z\frac{E}{z}dz\right]=z^{-1/2+E/\hbar}\ , \tag{3.15}$$

which indeed solves Eq. (3.14) exactly, for any value of E. Then, the single valuedness or analyticity condition selects $E=(k+\frac{1}{2})\hbar$, giving the eigenfunction $\psi_k(z)=z^k$, which is exact.

This trivial observation will help us clarify and numerically improve the behavior of the WKB method at low quantum numbers (see Secs. IV B and IV C).

E. Comparison with other semiclassical techniques

A consequence of Eq. (2.6) is a formula for the Husimi function[9] where $z=(q-ip)/\sqrt{2}$,

$$|\psi\rangle\langle\psi|_N(q,p)=e^{-|z|^2/\hbar}|\psi(z)|^2\ , \tag{3.16}$$

a much simpler relation than that of the Wigner function to the Schrödinger wave function, for instance. It is manifest upon this formula that the Bargmann wave function carries explicit phase information in addition to the information provided by the Husimi function.

Equation (2.6) also links the Bargmann representation to coherent-state decompositions[10] and the WKB approx-

imation to methods based on Gaussian wave packet superpositions.[12]

In the language of action-angle coordinates, the Bargmann wave function over the energy curve looks like a wave function in the angle variable. The semiclassical quantization in Bargmann variables has technical advantages similar to those presented by action-angle quantization without sharing the latter's axiomatic difficulties (about formulating the fully quantal theory in action-angle variables).

IV. THE WKB METHOD USING NORMAL ORDERING (REF. 1)

Normal ordering is very natural in the adapted Bargmann representation: it simply puts all differentiation operators (d/dz) to the right of all multiplication operators (z). We now describe WKB algorithms to solve $H\psi=E\psi$ in terms of the normal symbol $H_N(z,y)$, assuming now without real loss of generality that this symbol is $\hbar$ independent (purely classical).

A. The standard solutions

The WKB solution is most conveniently sought in the form

$$\psi(z)=\exp\left[\frac{1}{\hbar}\int^z\sum_{n=0}^{\infty}u_n(z')\hbar^n dz'\right] . \tag{4.1}$$

The leading term is, as usual,

$$u_0(z')=y_E(z') , \tag{4.2}$$

with

$$H_N(z',y_E(z'))=E . \tag{4.3}$$

Various algorithms can effectively compute the expansion coefficients u_n to any order n, as polynomials of $(\partial H_N/\partial y)^{-1}$ and of the other derivatives of H_N at $(z,y_E(z))$. Those algorithms can be performed by symbolic algebra computer programs. They are described in Appendix B.

To reach the same order of accuracy as Eq. (3.13), only u_0 and u_1 are needed, and the WKB solution of Appendix B then reduces to

$$\psi(z)\sim\exp\left[\frac{1}{\hbar}\int^z y_E(z')dz' + \frac{1}{2}\int^z\frac{\dfrac{\partial^2 H_N}{\partial y^2}\dfrac{\partial H_N}{\partial z}}{(\partial H_N/\partial y)^2}(z',y_E(z'))dz'\right] . \tag{4.4}$$

The quantization condition again expresses the analyticity of $\psi(z)$ inside the real energy curve, as

$$\oint\frac{\psi'}{\psi}dz=2\pi ik , \tag{4.5}$$

or

$$\sum_{n=0}^{\infty}\hbar^n\oint u_n dz=2\pi i\hbar k . \tag{4.6}$$

There appears no longer any explicit Maslov correction on the right-hand side. Here, this correction is distributed partly in the term $\oint u_1 dz$, and partly on the difference between the Weyl-ordered and normal-ordered operators. For the harmonic oscillator, $\exp(i/\hbar\int u_0 dz)$ is already the exact eigenfunction, and $u_1=u_2=\cdots=0$, so that the Maslov correction must be entirely accounted for by the shift from Weyl to normal ordering, which is a well-known fact in this case. Otherwise, all properties listed in Sec. III are valid here as well.

B. The optimized WKB method

Semiclassical analysis is not expected to give good quantitative predictions at low quantum numbers. Nevertheless, we shall show that by exploiting the lack of canonical invariance of normal ordering, the WKB method can be made much more accurate for the ground states (and low-lying excited states, as it seems), at the expense of only a slight deterioration for large quantum numbers. The idea is to select the normal ordering self-consistently by a variational Hartree argument.

If $H(q,p)$ is the Hamiltonian under consideration, assumed to be bounded below, we minimize the expectation value

$$\langle\Omega|H|\Omega\rangle \tag{4.7}$$

over all possible ground states of positive quadratic Hamiltonians (and their translates in phase space). Assuming uniqueness, we take the minimizing center under translations as new origin in phase space. The essential step is then to choose the minimizing quadratic Hamiltonian $h_{\min}$ as the reference oscillator for normal ordering and complex structure, i.e., $h_{\min}(z,z^*)=z^*z$.

The minimization conditions are given by self-consistent equations for the normal symbol in the final Bargmann representation itself:

$$\partial_z H_N(0,0)=\partial_{z^*}H_N(0,0)=0 \text{ (translation minimum)} \tag{4.8}$$

$$\left.\begin{aligned}&\partial_z^2 H_N(0,0)=\partial_{z^*}^2 H_N(0,0)=0 &(4.9)\\ &\omega=\partial_z\partial_{z^*}H_N(0,0)>0 &(4.10)\end{aligned}\right\} \text{ (general minimum) .}$$

Consequently, around $(z,z^*)=(0,0)$ we have

$$H_N(z,z^*)=H_N(0,0)+\omega z^*z+O(|z|^3) . \tag{4.11}$$

Now, $H_N(0,0)$ is the minimal expectation value, which is often a very good approximation to the exact ground state, as the practice of the Rayleigh-Ritz method indicates. In turn, the WKB method with respect to this normal ordering will yield levels very close to those of $H_N(0,0)+\omega\hbar zd/dz$ for low quantum numbers; in this regime it will resemble the random-phase approximation (RPA) expansion used in Hartree-Fock theory.[13] But for large quantum numbers it will work even better, since

this WKB method is still semiclassical. Consequently, this single method will be more uniformly accurate over the whole spectrum than either standard WKB or RPA expansion taken separately.

As a numerical example we consider the quartic oscillator:

$$H=-\frac{\hbar^2}{2}\frac{d^2}{dq^2}+q^4 . \tag{4.12}$$

The nontrivial part of the variational argument lies on minimizing the frequency Ω of the trial harmonic oscillator $h=\frac{1}{2}(p^2/\Omega+\Omega q^2)$. The corresponding symbols are [with $z=(\sqrt{\Omega}q-ip/\sqrt{\Omega})/\sqrt{2}$, $z^*=(\sqrt{\Omega}q+ip/\sqrt{\Omega})/\sqrt{2}$]

$$H_W=-\frac{\Omega}{4}(z-z^*)^2+\frac{1}{4\Omega^2}(z+z^*)^4 , \tag{4.13}$$

$$H_N=\exp\left[\frac{\hbar}{2}\partial_z\partial_{z^*}\right]H_W \tag{4.14}$$

[we have used Eq. (1.11)], hence

$$H_N=-\frac{\Omega}{4}(z-z^*)^2+\frac{1}{4\Omega^2}(z+z^*)^4 +\hbar\left[\frac{\Omega}{4}+\frac{3}{2\Omega^2}(z+z^*)^2\right]+\frac{3\hbar^2}{4\Omega^2} . \tag{4.15}$$

The crucial self-consistent equation is (4.9), giving

$$\Omega=(6\hbar)^{1/3} \tag{4.16}$$

and afterwards

$$H=6^{1/3}\hbar^{4/3}\left[\frac{3}{8}+z\frac{d}{dz}+\frac{1}{24}\left[z^4+4z^3\frac{d}{dz}+6z^2\frac{d^2}{dz^2} +4z\frac{d^3}{dz^3}+\frac{d^4}{dz^4}\right]\right] . \tag{4.17}$$

The correct scaling behavior of H with respect to $\hbar$ factorizes out, and it is the operator in the brackets (with an effective $\hbar=1$) which is then treated by the semiclassical formulas (4.1)–(4.6).

Table I shows the numerical comparison of the usual Bohr-Sommerfeld formula with Eq. (4.6) used in this optimized representation, to increasing orders in $\hbar$. We emphasize that the optimization has drastically changed the expansion parameter. This is most obvious in the extreme anharmonic case of Eq. (4.12), giving a frequency Ω in Eq. (4.16) highly nonanalytic in $\hbar$ at $\hbar=0$.

C. The localized or "descaled" WKB method

If the classical Hamiltonian has an absolute minimum $E_{\min}$, any standard WKB method becomes singular for $E=E_{\min}$. In the Bargmann representation, however, because the harmonic oscillator is trivial, the WKB method can be carried down to $E=E_{\min}$ by means of a simple scale transformation.

We choose the normal ordering scheme, for instance. We can always assume that the classical minimum is $E_{\min}=0$ at $q=p=0$. The scale transformation is a change of variable $z\to z'$:

$$z=\sqrt{\hbar}z', \quad \hbar d/dz=\sqrt{\hbar}d/dz' ,$$

which essentially blows up to a macroscopic scale a phase-space disk of radius $\sqrt{\hbar}$ around the minimum. The quantum Hamiltonian expansion around the minimum has then the form

$$H=\hbar\omega z'\frac{d}{dz'}+\sum_{n=3}^{\infty}\hbar^{n/2}\left[\sum_{j+k=n}\frac{1}{j!k!}\frac{\partial^j}{\partial z^j}\frac{\partial^k}{\partial y^k}H_N\right]\Bigg|_{z=y=0} \times z'^j\left[\frac{d}{dz'}\right]^k . \tag{4.18}$$

The spirit of the WKB method is then to look for

TABLE I. Numerical comparison of the ordinary (a) and optimized (b) Bohr-Sommerfeld quantization rules for the eigenvalues E_k of the quartic oscillator $-\frac{1}{2}d^2/dq^2+q^4$. In both cases, in order to avoid inverting the quantization formulas, we treated the quantum numbers $k=0,1,2,\ldots$ as the unknown quantities and used as input the tabulated energy levels E_k. One should compare to the exact k the values $k_{(n)}$ obtained by n-term truncations of the Bohr-Sommerfeld series. In (a) we used the standard rule equivalent to Eq. (3.6) with corrections (Ref. 20); these naturally jump by two orders at each step; no improvement is obtained for the lowest three states at higher orders (values not shown). In (b) we applied Eq. (4.6) to the Hamiltonian (4.17). Considerable improvement is gained for the ground state at the expense of a slight decrease in convergence for large quantum numbers, which means a more uniform accuracy.

	(a) Ordinary				(b) Optimized			
k	E_k	$k_{(1)}$	$k_{(3)}$	k	$k_{(0)}$	$k_{(1)}$	$k_{(2)}$	$k_{(3)}$
0	0.667 986 259	0.081	0.0358	0	−0.0074	−0.0093	−0.010	−0.0005
1	2.393 644 02	1.014	0.9967	1	0.815	0.9519	0.984	0.9947
2	4.696 795 39	2.010	1.999 97	2	1.728	1.959	1.993	1.9997
3	7.335 730 01	3.007	2.999 94	3	2.660	2.962	2.995	2.999 96
4	10.244 308 5	4.006	3.999 976	4	3.603	3.965	3.997	4.000 05
5	13.379 336 6	5.005	4.999 987	5	4.553	4.967	4.997	5.000 07
6	16.711 889 6	6.004	5.999 992	6	5.509	5.968	5.9978	6.000 07
7	20.220 849 5	7.0035	6.999 995	7	6.468	6.970	6.9981	7.000 07
8	23.889 993 7	8.0031	7.999 997	8	7.431	7.971	7.9984	8.000 06
9	27.706 393 5	9.0028	8.999 998	9	8.397	8.972	8.9986	9.000 05
10	31.659 456 6	10.0025	9.999 998	10	9.364	9.973	9.9988	10.000 04

eigenfunctions of the Hamiltonian $\hbar^{-1}H$, in the form

$$\Phi(z')=\exp\int^{z'} v(\hbar;z'')dz'' \ . \tag{4.19}$$

The nonlinear equation for v can be solved by iteration, giving

$$v(\hbar;z'')=\frac{E'}{z''}+\sum_{n\geq 1}\hbar^{n/2}P_n\left[z'',\frac{1}{z''},E'\right] \tag{4.20}$$

where $E'=\hbar^{-1}E$ is the unknown eigenvalue and P_n is a polynomial.

Then the quantization condition (4.5) in terms of the function v simply expresses that the residue of v, i.e., the coefficient of $1/z''$ in Eq. (4.20), should be a non-negative integer k. To lowest order, this gives $E'=k$, and the corrections to this form a power series in $\hbar^{1/2}$. But this power series can also be generated by linear quantum perturbation theory (the Rayleigh-Schrödinger method) applied around the unperturbed Hamiltonian $\hbar\omega zd/dz$.[14] Hence, upon this descaling, the WKB algorithm becomes equivalent to standard perturbation theory in an obvious fashion. The so-descaled WKB expansion is therefore positively weaker than the original WKB expansion, all the more that the quantum number k is larger; the original WKB expansion can conversely be viewed as a partially resummed perturbation series. The main advantage of the descaled method is that, being just perturbation theory from a different perspective, it readily extends to any number of degrees of freedom, requiring no additional constants of the motion in contrast with the ordinary WKB method (see Conclusion).

CONCLUSION

We shall only observe in conclusion that the Bargmann representation is also more promising for a unified WKB treatment of several classes of quantum Hamiltonians in l degrees of freedom ($l>1$). Completely integrable systems are handled by the same algebra as in the Schrödinger representation;[4,1] multidimensional extensions of Eqs. (3.3) and (3.6) give the joint eigenstates and eigenvalues of a collection of commuting constants of the motion, again with all caustic crossings avoided. But in the Bargmann representation, we can also treat systems with fewer constants of the motion but with one stable fixed point per degree of freedom corresponding to a missing constant. The best example is the quantization of a system with a classically stable orbit isolated in its energy surface.[15] The longitudinal motion, generated by the conserved Hamiltonian itself, can be quantized by a standard WKB approach, and small transversal motion can be quantized by the descaled WKB approach. The fact that the two types of motion are globally coupled is no obstacle. An output of the treatment is the analog of the Bohr-Sommerfeld quantization formula for such an isolated orbit (see Refs. 16 and 4 for details, Ref. 1 for the treatment in Bargmann variables).

This generalization allows the WKB method in the Bargmann representation to cover certain quasi-integrable systems. At the other extreme, for very irregular or chaotic systems, the intrinsic structure of the eigenstates leaves little hope that their state vectors will admit any WKB description at all. In this case, we do not expect that such a difficulty is curable by way of a change of representation (see, however, Ref. 17 for a more optimistic point of view).

Note added. J. Kurchan, P. Leboeuf, and M. Saraceno have independently developed similar results in a framework which moreover encompasses curved phase spaces associated with symmetry groups SU(2) and SU(1,1), thus considerably enlarging the scope of the method.[18]

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APPENDIX A: WKB EIGENFUNCTIONS TO ALL ORDERS IN WEYL CALCULUS (REFS. 5 AND 1)

We describe a semiclosed WKB expression which solves to any order in $\hbar$ the operator equation $H\psi=E\psi$ in one degree of freedom, using the Weyl symbol H_W, which we assume to be $\hbar$ independent until the last paragraph.

The key idea is to solve the operator equation

$$(2\pi\hbar)^{-1}|\psi\rangle\langle\psi|=(2\pi i)^{-1}\times\lim_{\epsilon\searrow 0}\left[\frac{1}{H-E-i\epsilon}-\frac{1}{H-E+i\epsilon}\right]$$
$$[\equiv\delta(H-E)] \tag{A1}$$

in power series of $\hbar$ for the Weyl symbols. We must assume that on the right-hand side, the limits $\epsilon\searrow 0$ and $\hbar\to 0$ commute (*this* will fail in higher dimensions); and that on the left-hand side, ψ is given by a WKB ansatz:

$$\psi(q)=ae^{iS/\hbar} \text{ with } a,S \text{ real} \ . \tag{A2}$$

(We now use real coordinates and the Schrödinger representation because the algorithm is easier to comprehend this way, but the algebraic results go over to the Bargmann case by canonical invariance.)

The Wigner function is then

$$|\psi\rangle\langle\psi|_W(\hbar;q,p)=\int a(q-r/2)a(q+r/2)e^{(i/\hbar)[S(q-r/2)-S(q+r/2)+pr]}dr \ . \tag{A3}$$

We describe the computation to lowest order in $\hbar$ first.

We expand the integrand around the point $(p=dS/dq, r=0)$, which is where its phase variation is slowest, being

$$\delta S(q,r)=S(q-r/2)-S(q+r/2)+p(q)r=O(r^3)\ . \tag{A4}$$

We may then neglect δS and the amplitude variation around $r=0$, and we find

$$(2\pi\hbar)^{-1}|\psi\rangle\langle\psi|_W \sim (2\pi\hbar)^{-1}a(q)^2\int e^{(i/\hbar)[-(dS/dq)r+pr]}dr$$
$$=a(q)^2\delta(p-dS/dq)\ . \tag{A5}$$

On the other side, to lowest order in $\hbar$, we have (locally)

$$[\delta(H-E)]_W \sim \delta(H_W(q,p)-E)$$
$$=(\partial H_W/\partial p_E)^{-1}\delta(p-p_E(q)) \tag{A6}$$

where we had to change the independent variable under the delta distribution [using $H_W(q,p_E(q))=E$], so that we may now readily compare Eq. (A6) with (A5). We thus obtain

$$\frac{dS}{dq}=p_E(q) \quad \text{or} \quad S(q)=\int^q p_E(q')dq' \tag{A7}$$

by identifying the distributions' supports, and

$$a(q)=\left[\frac{\partial H_W}{\partial p_E}\right]^{-1/2} \tag{A8}$$

by identifying their intensities.

We have thus recovered the lowest-order WKB solution in a seemingly tortuous way, but now the incorporation of quantum corrections is immediate. Indeed, if the functions a and S in Eq. (A2) have full real expansions

$$a\sim\sum_0^\infty a_n(q)\hbar^n,\quad S=\sum_0^\infty S_n(q)\hbar^n\ , \tag{A9}$$

then the analog of Eq. (A5) is

$$(2\pi\hbar)^{-1}|\psi\rangle\langle\psi|_W \sim a(q)^2\left[\delta(p-p_E(q))+[p_E(q)-dS/dq]\delta'(p-p_E(q))+\sum_{s=2}^\infty \varphi_s(q)\delta^{(s)}(p-p_E(q))\right]\ , \tag{A10}$$

with coefficients $\varphi_s(q)$ which will not be needed.

On the other hand, the full expansion of Eq. (A6) is[5]

$$[\delta(H-E)]_W=\sum_{r=0}^\infty \frac{1}{r!}\mathcal{G}_r^W(\hbar;q,p)\delta^{(r)}(H_W(q,p)-E)\ , \tag{A11}$$

with

$$\mathcal{G}_r^W(\hbar;q,p)=\{[H-H_W(q,p)\cdot\mathbb{1}]^r\}_W(\hbar;q,p) \tag{A12}$$

where $\mathbb{1}$ is the identity operator; then the change to p as independent variable inside (A11) results in

$$[\delta(H-E)]_W=\sum_{s=0}^\infty \alpha_s^W(\hbar;q)\delta^{(s)}(H_W(q,p)-E) \tag{A13}$$

where

$$\alpha_s^W(\hbar;q)=\int[\delta(H-E)]_W[p-p_E(q)]^s/s!\,dp$$
$$=\sum_{r=s}\frac{(-1)^r}{r!}\left[(H_W)_p^{-1}\frac{\partial}{\partial p}\right]^r$$
$$\times\left[(H_W)_p^{-1}\frac{[p_E(q)-p]^s}{s!}\mathcal{G}_r^W(\hbar;q,p)\right]\Bigg|_{p=p_E(q)}\ . \tag{A14}$$

Finally, the comparison of Eqs. (A10) and (A13) yields the full WKB phase and amplitude, respectively, as

$$S=\int^q(p_E-\alpha_1^W/\alpha_0^W)(q')dq',\quad a=(\alpha_0^W)^{1/2}\ . \tag{A15}$$

This is an effective formula to any finite order $\hbar^n$ because the sums (A11) and (A14) are then finite, due to the property[5]

$$\mathcal{G}_r^W=o(\hbar^n)\ \text{ for any } r>3n/2\ . \tag{A16}$$

Moreover, $\mathcal{G}_r^W$ and α^W only contain *even* powers of $\hbar$. Now, the Bargmann analogs are obtained by the substitutions $q\to z$, $p\to y$, $\hbar\to i\hbar$ (see Sec. III A). For instance (still with $\hbar$-independent H_W),

$$\mathcal{G}_0^W\equiv 1,\quad \mathcal{G}_1^W\equiv 0\ ,$$
$$\mathcal{G}_2^W=[(H_W)_{zy}^2-(H_W)_{zz}(H_W)_{yy}]\hbar^2/4+O(\hbar^4)\ ,$$
$$\mathcal{G}_3^W=[(H_W)_z^2(H_W)_{yy}-2(H_W)_z(H_W)_y(H_W)_{zy}$$
$$+(H_W)_y^2(H_W)_{zz}]\hbar^2/4+O(\hbar^4)\ , \tag{A17}$$
$$\mathcal{G}_4^W=\mathcal{G}_5^W=\ldots=O(\hbar^4)$$

(subscripts denote differentiations), and

$$\alpha_0^W(z)=(\partial H_W/\partial p_E)^{-1}+O(\hbar^2),\quad \alpha_1^W=O(\hbar^2)\ , \tag{A18}$$

but here the $\hbar^2$ corrections are already so long that we do not reproduce them (23 terms for α_0, 13 terms for α_1). This algebraic complexity is the one practical disadvantage of the Bargmann representation, as the Hamiltonian no longer enjoys a privileged simple form like $p^2+V(q)$ in real coordinates. However, symbolic computer languages can easily manipulate such bulky expressions.[19]

Finally, when the Weyl symbol itself contains $\hbar$-dependent terms, they can be taken into account in two equivalent ways: either by using the same formulas [(A11)–(A15)] but reexpanding H_W and $p_E(q)$ in powers of $\hbar$, or by using the classical limit H_0 everywhere in place of H_W (which redefines the coefficients $\mathcal{G}_r^W$ and α_s^W).

APPENDIX B: WKB EIGENFUNCTIONS TO ALL ORDERS IN NORMAL-ORDERED CALCULUS (REF. 1)

We describe four possible algorithms for computing the WKB solutions of the eigenstate equation $H\psi=E\psi$ in terms of the normal symbol $H_N(z,y)$, which we assume to be $\hbar$ independent until the last paragraph.

(1) An obvious but indirect method is to return to the Weyl symbol, using the inverse of Eq. (1.11) or (4.14) (the latter in complex coordinates), i.e., $H_W(\hbar;z,y)=\exp(-\hbar/2\partial_z\partial_y)H_N(z,y)$. To the order in $\hbar$ corresponding to Eq. (3.13), this simplifies as

$$H_W(\hbar;z,y)\sim H_N(z,y)-\frac{\hbar}{2}(H_N)_{zy} \tag{B1}$$

(subscripts will denote differentiations), and the eigenfunction itself is

$$\psi\sim\left[\frac{\partial H_W}{\partial y}\right]^{-1/2}_{y=Y_E}\exp\left[\frac{1}{\hbar}\int^z Y_E(\hbar;z')dz'\right], \tag{B2}$$

where Y_E is given by

$$H_W(\hbar;z,Y_E(z))=E\ . \tag{B3}$$

We shall use in fact Eq. (B2) in the form

$$\hbar\frac{d}{dz}\ln\psi\sim Y_E(\hbar;z)-\frac{\hbar}{2}\frac{d}{dz}\ln\left[\frac{\partial H_W}{\partial y}\right]\Bigg|_{y=Y_E}. \tag{B4}$$

To that same order of accuracy, we can further simplify,

$$Y_E(\hbar;z)\sim Y_E(z)+\frac{\hbar}{2}\frac{(H_N)_{xy}}{(H_N)_y}\Bigg|_{y=Y_E(z)}, \tag{B5}$$

and

$$\hbar\frac{d}{dz}\ln\psi\sim\left[y_E(z)+\frac{\hbar}{2}\frac{(H_N)_{zy}}{(H_N)_y}\right]-\frac{\hbar}{2}\frac{d}{dz}\ln(H_N)_y$$
$$\sim y_E(z)+\frac{\hbar}{2}\frac{(H_N)_z(H_N)_{yy}}{(H_N)_y^2}\ , \tag{B6}$$

where we have used

$$\frac{d}{dz}=\frac{\partial}{\partial z}-\frac{(H_N)_z}{(H_N)_y}\frac{\partial}{\partial y}\Bigg|_{y=y_E(z)}. \tag{B7}$$

Consequently, we obtain the WKB eigenfunction as given in Eq. (4.4),

$$\psi(z)\sim\exp\left[\frac{1}{\hbar}\int^z\left[y_E(z')+\frac{\hbar}{2}\frac{(H_N)_z(H_N)_{yy}}{(H_N)_y^2}(z',y_E(z'))\right]dz'\right].$$

To obtain higher orders we may then use Appendix A (including the last paragraph, since H_W depends explicitly on $\hbar$).

(2) We may adapt the same argument as in Appendix A to the case of the ordering where p operators are put to the right of q operators (in real coordinates) (Ref. 1, Part IV, Annex C), then transpose to complex coordinates using $q\to z$, $p\to y$, $\hbar\to i\hbar$. The analog of Eq. (A15) is then obtained as

$$\psi=\exp\left[\frac{1}{\hbar}\int^z\left[y_E-\frac{\alpha_1^N-\hbar d\alpha_0^N/dz'}{\alpha_0^N}\right](z')dz'\right], \tag{B8}$$

where total differentiation is in the sense of Eq. (B7), and

$$\alpha_s^N(\hbar;z)=\sum_{r=s}^{\infty}\frac{(-1)^r}{r!}\left[\left[(H_N)_y^{-1}\frac{\partial}{\partial y}\right]^r(H_N)_y^{-1}\frac{[y_E(z)-y]^s}{s!}\mathcal{G}_r^N(\hbar;z,y)\right]_{y=y_E(z)}, \tag{B9}$$

with

$$\mathcal{G}_r^N(\hbar;z,y)=\{[H-H_N(z,y)\mathbb{1}]^r\}_N(\hbar;z,y)\ , \tag{B10}$$

$$\mathcal{G}_r^N=o(\hbar^n)\ \text{ for any } r>2n\ . \tag{B11}$$

Thus Eq. (B8) is a semiclosed expression valid to any finite order in $\hbar$. To lowest order, for instance,

$$\alpha_0^N\sim(H_N)_y^{-1}+\frac{\hbar}{2}[(H_N)_y^{-2}(H_N)_{zyy}-(H_N)_y^{-3}(H_N)_{yy}(H_N)_{zy}]_{y=y_E(z)}\ ,$$
$$\alpha_1^N\sim\frac{\hbar}{2}[-2(H_N)_y^{-2}(H_N)_{zy}+(H_N)_y^{-3}(H_N)_z(H_N)_y^2]_{y=y_E(z)}\ , \tag{B12}$$

and Eq. (B8) reduces to Eq. (4.4).

The last two algorithms are iterative.

(3) Take as unknown function $v(\hbar;z)$ where

$$\psi(z)=\exp\left[\frac{1}{\hbar}\int^z y_E(z')\exp\left[\int^z v(\hbar;z')dz'\right]\right]. \tag{B13}$$

The eigenfunction equation $H\psi=E\psi$ then becomes

$$[H_N(z,y_E(z)+\hbar\partial_z)-E]\exp\left[\int^z v(\hbar;z')dz'\right]=0\ . \tag{B14}$$

This has the Taylor expansion

$$\sum_{n=1}^{\infty}\frac{1}{n!}(H_N)_{y^n}[y_E(z)-y\cdot\mathbb{1}+\hbar d/dz]^n\exp\left[\int^z v(\hbar;z')dz'\Big|_{y=y_E(z)}\right]=0\ . \tag{B15}$$

Now, we have that

$$\hbar^{-1}\exp\left[-\int^z v(\hbar;z')dz'\right][y_E(z)-y\cdot\mathbb{1}+\hbar d/dz]^n\exp\left[\int^z v(\hbar;z')dz'\right]\Big|_{y=y_E(z)}=\mathcal{P}_n(\hbar;v(z),dv/dz,d^2v/dz^2,\ldots)\ , \tag{B16}$$

is a certain polynomial in $\hbar$, v, and its derivatives at z (the coefficients of $\mathcal{P}_n$ depending on derivatives of H_N). In particular,

$$\mathcal{P}_1=v,\quad \mathcal{P}_2=-\frac{(H_N)_z}{(H_N)_y}+\hbar\left[\frac{dv}{dz}+v(z)^2\right]\ . \tag{B17}$$

Therefore Eq. (B15) can be rewritten as

$$v(\hbar;z)=-(H_N)_y^{-1}\sum_{n=2}^{\infty}\frac{1}{n!}(H_N)_{y^n}\mathcal{P}_n(\hbar;v(z),dv/dz,\ldots)\ . \tag{B18}$$

The right-hand side can be made explicit to any finite order in $\hbar$ (it is then analogous to the Riccati equation in the Schrödinger case). Equation (B18) can then be solved to that finite order by repeated iterations.

The first two steps give $v_{(0)}=0$, and

$$v_{(1)}=+\frac{(H_N)_{yy}(H_N)_z}{2(H_N)_y^2}\ , \tag{B19}$$

which corresponds to Eq. (4.4).

(4) The last algorithm resembles the descaling method described in Sec. IV C but now the expansion is performed around a regular point (z_0,y_0) on the classical orbit, i.e., a new variable z' is used, where

$$z=z_0+\sqrt{\hbar}z',\quad \hbar\frac{d}{dz}=y_0+\sqrt{\hbar}\frac{d}{dz'}\quad [H_N(z_0,y_0)=E]\ . \tag{B20}$$

The eigenfunction in the new variable is

$$\psi(z)\equiv\exp(y_0z/\sqrt{\hbar})\tilde{\psi}(z')\ . \tag{B21}$$

As in the preceding algorithm we write the equation in terms of $\tilde{v}=(d/dz)\ln\tilde{\psi}$. It reads in expanded form as

$$\exp\left[-\int^{z'}\tilde{v}\right]\left[H_N(z_0,y_0)-E+\hbar^{1/2}\left[(H_N)_{z_0}z'+(H_N)_{y_0}\frac{d}{dz'}\right]+\sum_{m+n=2}^{\infty}\frac{(H_N)_{z_0^m}(H_N)_{y_0^n}}{m!n!}\hbar^{(m+n)/2}z'^m\left[\frac{d'}{dz}\right]^n\right]\exp\left[\int^{z'}\tilde{v}\right]=0\ . \tag{B22}$$

Since $H_N(z_0,y_0)=E$, the leading contribution comes from the linearized motion around the classical orbit, which is a well-known idea in semiclassical theory. Rewritten accordingly, as

$$\tilde{v}(z')=-\frac{(H_N)_{z_0}}{(H_N)_{y_0}}z'+\sum_{m+n=2}^{\infty}\hbar^{(m+n-1)/2}\frac{(H_N)_{z_0^m}}{m!}\frac{(H_N)_{y_0^n}}{n!}z'^m\left[\exp\left[-\int^{z'}\tilde{v}\right]\left[\frac{d}{dz'}\right]^n\exp\left[\int^{z'}\tilde{v}\right]\right]\ , \tag{B23}$$

Eq. (B22) can be solved by repeated iterations of Eq. (B23). This algorithm is a close relative of the previous one, giving the function v in Eq. (B13) as

$$v(\hbar;z_0,y_0)=\hbar^{-1/2}\tilde{v}(z'=0)\ , \tag{B24}$$

and it has the most suitable form for extensions to multidimensional systems in conjunction with the descaled method around a fixed point.[1]

(5) Finally, to account for quantum corrections coming from an *explicit* dependence in $\hbar$ of the normal symbol H_N itself, the same formulas can be used, provided all $\hbar$-dependent quantities, like H_N and now also $y_E(z)$, are further reexpanded. For the second algorithm, the alternative described in the last sentence of Appendix A can equally well be used.

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