Semiclassical approximations in the coherent-state representation

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We analyze the semiclassical limit of the stationary Schrödinger equation in the coherent-state representation simultaneously for the groups W_1, SU(2), and SU(1,1). A simple expression for the first two orders for the wave function and the associated semiclassical quantization rule is obtained if a definite choice for the classical Hamiltonian and expansion parameter is made. The behavior of the modulus of the wave function, which is a distribution function in a curved phase space, is studied for the three groups. The results are applied to the quantum triaxial rotor.

I. INTRODUCTION

In recent years there has been a renewed interest in semiclassical approximations in many fields of physics. Two aspects arise which are not generally recognized in the standard textbook WKB approach and which are at the root of this interest. The first is the understanding that many quantum theories possess a classical limit—different from the standard $\hbar \to 0$ limit—when a certain parameter N (e.g., the dimension of the space, of the group representation, etc.) goes to infinity. These limits, broadly known as $1/N$ expansions,[1] can provide a wealth of information about many aspects of otherwise intractable quantum problems.

The second aspect, much more fundamental and difficult, is related to the fact that most classical limits obtained in this way lead to nonintegrable classical dynamics and to the awareness that the ensuing chaotic motion severely limits the applicability of standard semiclassical methods.

The semiclassical limit of the Schrödinger equation in this case is not yet completely understood and is a subject of current research.[2] The integrable case when the limit is the standard $\hbar \to 0$ has been extensively studied (usually in the coordinate representation) and corresponds of course to the WKB approximation.[3]

In this paper we address mainly the first aspect and show how WKB works for phase spaces associated to groups other than the W_1 Weyl group. A detailed analysis for the case of the Weyl group is carried out in Ref. 4, and we will frequently refer the reader throughout this paper to that reference.

We use the coherent-state representation which due to its analyticity properties provides a smooth, global approximation to the semiclassical wave functions. There are no caustics and all the relevant quantities are displayed in phase space.[5,6,4] In the case of the Weyl group this representation takes the form of a Hilbert space of analytic functions studied extensively by Bargmann,[7] but it is also available for many other groups. In fact, coherent states are known[8] for a large number of semisimple (both compact and noncompact) and nilpotent groups. We will be interested here in conservative one-dimensional systems belonging to the representative cases of the Weyl W_1, SU(2), and SU(1,1) groups, using a formalism that allows for their unified treatment.

The group structure induces its own geometry on the space of parameters that label the coherent states—this space corresponds to a manifold $\mathcal{M}$ which has a symplectic structure defined on it and therefore can be thought of as a "curved" phase space.

Quantum mechanics defined in the unitary representations of these groups goes to a classical mechanics on the respective phase spaces when the weight of the representation becomes large. This limit has been studied before mainly using path-integral methods.[9–11]

Our strategy is different here; we follow closely the standard WKB approach of quantum-mechanical textbooks. We first write the differential version of the stationary Schrödinger equation in the coherent-state representation valid for the three groups. This equation contains the weight of the unitary representation as a parameter and therefore using a rather standard argument we construct the asymptotic solution—which we study to next-to-leading order.

There are several possible "classical" Hamiltonians (symbols) defined on $\mathcal{M}$ associated with a given quantum Hamiltonian, the most usual ones being the Q and P symbols[8,9] (related in the W_1 case to normal and antinormal ordering, respectively). The quantization condition arises from the requirement of analyticity[12,5] and takes the form of a Bohr-Sommerfeld quantization rule.

Because each type of symbol possesses a different dependence in the semiclassical parameter, the form of this quantization condition depends on the symbol under use. Which symbol yields better results depends on the particular problem under consideration. The central result of this paper is to show that there is a unified geometrical treatment underlying the semiclassical approximation in many group representations, therefore extending considerably the application of methods available for the Weyl group[5] in these more general limits. Specifically,

we study the wave functions and quantization rules and their next-to-leading-order corrections for the groups W_1, SU(2), and SU(1,1). We find that the corrections are greatly simplified if the following points are true.

(i) These specific choices are made for the expansion parameter: $\hbar$ for the Weyl group, $(j+\frac{1}{2})^{-1}$ for the SU(2) group, and $(k-\frac{1}{2})^{-1}$ for the SU(1,1) group (j and k being the usual labels of the representation). The convenience of such choices for the expansion parameters is also suggested in other contexts: $(j+\frac{1}{2})^{-1}$ in the Langer correction[13] for the radial Schrödinger equation and $(k-\frac{1}{2})^{-1}$ in the case of the free motion of a particle on a manifold of negative constant curvature.[14]

(ii) An "intermediate" symbol (located between Q and P) is used as classical Hamiltonian. This symbol coincides with the usual classical Weyl-Wigner[15] symbol in the case of the W_1 group. In the case of SU(2) and SU(1,1) groups, this intermediate symbol coincides to this order with the generalization of the Weyl-Wigner symbol as given by Berezin.[16]

As in ordinary Maslov-Einstein-Brillouin-Keller treatments[17] the next-to-leading order enters through a Maslov index which, under certain assumptions, depends *only on the nature of the stationary points encircled by the trajectory.*

We also study the square amplitude of the wave function in the coherent-state representation, which provides a positive definite distribution in the phase space $\mathcal{M}$, in many ways similar to the Wigner distribution.[15] There are important differences, however, since, as is known, besides being positive definite this distribution is smooth and converges onto classical invariant structures. It constitutes therefore an ideal tool for the identification of these structures in quantum eigenfunctions. For the case of the Weyl group, this distribution was first used by Husimi[18] and its semiclassical limit studied by Takahashi.[19] We generalize these results for the other groups.

The paper is organized as follows. In Sec. II we review the coherent states of W_1, SU(2), and SU(1,1) introducing a unified notation. In Sec. III we obtain the asymptotic limit up to next-to-leading order for the stationary Schrödinger equation. In Sec. IV we study the analyticity requirements that lead to quantization including the Maslov correction. In Sec. V we study the square modulus of the wave functions and show how it converges smoothly onto the classical trajectories of a Hamiltonian which is somewhere in between the classical Q and P symbols. Finally as an illustration we apply in Sec. VI the results to the simple case of the asymmetric quantum rotor.

II. COHERENT STATES

In this section we review briefly the properties of coherent states, in particular their use as a phase-space representation (the Bargmann representation). Excellent and very comprehensive reviews of coherent states, their properties, and applications have appeared recently in the literature.[8,9]

The emphasis will be to show that well-known results for the usual coherent states of the harmonic oscillator can be easily extended to coherent states of other groups and to present a unified treatment for the elementary groups W_1, SU(2), and SU(1,1).

A. The elementary groups

1. The Weyl group W_1

The generators are a, $a^\dagger$, and I with commutation relations

$$[a,a^\dagger]=(1/\hbar)I\ ,\qquad [a,I]=[a^\dagger,I]=0\ . \tag{2.1}$$

Notice the slightly unconventional placement of $\hbar$ in (2.1) which results from our definition of a and $a^\dagger$ in terms of the classical operators $\hat{p}$ and $\hat{q}$:

$$a=\frac{1}{\sqrt{2\hbar}}\left[\sqrt{m\omega}\hat{q}+i\frac{1}{\sqrt{m\omega}}\hat{p}\right]\ ,\qquad a^\dagger=\frac{1}{\sqrt{2\hbar}}\left[\sqrt{m\omega}\hat{q}-i\frac{1}{\sqrt{m\omega}}\hat{p}\right]\ . \tag{2.2}$$

This normalization allows a uniform treatment of all groups.

The coherent states are defined as

$$|z\rangle=\exp(\bar{z}a^\dagger)|0\rangle\ ,\qquad a|0\rangle=0 \tag{2.3}$$

where z (and its complex conjugate $\bar{z}$) are classical phase-space coordinates

$$z=\frac{1}{\sqrt{2}}\left[\sqrt{m\omega}q-i\frac{1}{\sqrt{m\omega}}p\right]\ ,\qquad \bar{z}=\frac{1}{\sqrt{2}}\left[\sqrt{m\omega}q+i\frac{1}{\sqrt{m\omega}}p\right]\ . \tag{2.4}$$

The norm of $|z\rangle$ is given by

$$\langle z|z\rangle=\exp(z\bar{z}/\hbar) \tag{2.5}$$

and the algebra is realized by the differential operators:

$$\langle z|a|\psi\rangle=\frac{d}{dz}\langle z|\psi\rangle\ ,\qquad \langle z|a^\dagger|\psi\rangle=\frac{1}{\hbar}z\langle z|\psi\rangle\ . \tag{2.6}$$

The Hilbert space of analytic functions where a and $a^\dagger$ are Hermitian conjugates has been extensively studied by Bargmann.[7]

2. The SU(2) group

The generators are $J_\pm$ and J_0 with the algebra

$$[J_0,J_\pm]=\pm J_\pm\ ,\qquad [J_-,J_+]=-2J_0\ . \tag{2.7}$$

The orthonormal bases of the unitary representations are labeled by the quantum numbers j and m and they

span the Hilbert space which is finite and $2j+1$ dimensional. Coherent states for a given j representation are defined as

$$|z\rangle=\exp(\bar{z}J_+)|0\rangle \tag{2.8}$$

where $|0\rangle$ is the lowest weight state $|j,-j\rangle$.

The norm is given by

$$\langle z|z\rangle=(1+z\bar{z})^{2j} \tag{2.9}$$

and the generators can be represented as differential operators

$$\begin{aligned}\langle z|J_+|\psi\rangle&=\left[-z^2\frac{d}{dz}+2jz\right]\langle z|\psi\rangle\ ,\\ \langle z|J_-|\psi\rangle&=\frac{d}{dz}\langle z|\psi\rangle\ ,\\ \langle z|J_0|\psi\rangle&=\left[z\frac{d}{dz}-j\right]\langle z|\psi\rangle\ .\end{aligned} \tag{2.10}$$

The Hilbert space is here that of polynomials of degree $2j+1$.

3. *The SU(1,1) group*

The generators are $K_\pm$ and K_0 with the algebra

$$\begin{aligned}&[K_0,K_\pm]=\pm K_\pm\ ,\\ &[K_-,K_+]=2K_0\ .\end{aligned} \tag{2.11}$$

As the group is not compact, unitary representations are infinite dimensional. We will only consider here the discrete representations D^k_+. Coherent states are defined as

$$|z\rangle=\exp(\bar{z}K_+)|0\rangle \tag{2.12}$$

where $|0\rangle$ is the lowest weight state of the D^k_+ representation defined as

$$\begin{aligned}&K^2|0\rangle=k(k-1)|0\rangle\ ,\\ &K_0|0\rangle=k|0\rangle\end{aligned} \tag{2.13}$$

where $K^2=K_0^2-\frac{1}{2}(K_+K_-+K_-K_+)$. The norm is

$$\langle z|z\rangle=(1-z\bar{z})^{-2k} \tag{2.14}$$

and a differential realization of (2.11) is given by

$$\begin{aligned}\langle z|K_+|\psi\rangle&=\left[z^2\frac{d}{dz}+2kz\right]\langle z|\psi\rangle\ ,\\ \langle z|K_-|\psi\rangle&=\frac{d}{dz}\langle z|\psi\rangle\ ,\\ \langle z|K_0|\psi\rangle&=\left[z\frac{d}{dz}+k\right]\langle z|\psi\rangle\ .\end{aligned} \tag{2.15}$$

B. Geometrical structures

It is convenient at this point to introduce a unified notation that will allow the simultaneous study of the three groups. For that purpose, we introduce parameters α and Ω which have the following values:

$$\alpha=\begin{cases}0 & \text{for } W\\ 1 & \text{for SU(2)}\\ -1 & \text{for SU(1,1)}\ ,\end{cases}\qquad \Omega=\begin{cases}1/\hbar & \text{for } W_1\\ 2j & \text{for SU(2)}\\ 2k & \text{for SU(1,1)}\end{cases} \tag{2.16}$$

and define

$$\lambda=\Omega+\alpha\ . \tag{2.17}$$

It will be shown in the following sections that λ is for the three groups the most "natural" semiclassical expansion parameter. In terms of these parameters the norm of the coherent states is

$$\langle z|z\rangle=(1+\alpha z\bar{z})^{\Omega/\alpha}=(1+\alpha z\bar{z})^{\lambda/\alpha-1}\ . \tag{2.18}$$

In the case of the Weyl group, (2.5) is obtained from (2.18) in the limit $\alpha\to 0$.

All the geometrical quantities associated with the manifold $\mathcal{M}$ spanned locally by the complex coordinates z and $\bar{z}$ can be expressed in terms of the quantity

$$F(z,\bar{z})=\frac{1}{\alpha}\ln(1+\alpha z\bar{z})=\frac{1}{\Omega}\ln\langle z|z\rangle\ . \tag{2.19}$$

We will also need the definition

$$\xi(z,\bar{z})\equiv\frac{\partial F}{\partial z}=\bar{z}/(1+\alpha z\bar{z})\ . \tag{2.20}$$

The metric is given by

$$d^2s=4\frac{\partial^2F}{\partial z\,\partial\bar{z}}dz\,d\bar{z}=4(1+\alpha z\bar{z})^{-2}dz\,d\bar{z}\ . \tag{2.21}$$

The corresponding two form ($\times$ denotes the exterior product)

$$\omega=2i\frac{\partial^2F}{\partial z\,\partial\bar{z}}dz\times d\bar{z} \tag{2.22}$$

defines the area on $\mathcal{M}$. For the Weyl group (2.22) can also be written in terms of p and q variables as [cf. (2.4)]

$$\omega=2dp\times dq\ .$$

Finally, a symplectic structure is defined for functions on $\mathcal{M}$ as

$$\begin{aligned}\{f,g\}&=i\left[\frac{\partial^2F}{\partial z\,\partial\bar{z}}\right]^{-1}\left[\frac{\partial f}{\partial z}\frac{\partial g}{\partial\bar{z}}-\frac{\partial f}{\partial\bar{z}}\frac{\partial g}{\partial z}\right]\\ &=i\left[\frac{\partial f}{\partial z}\frac{\partial g}{\partial\xi}-\frac{\partial f}{\partial\xi}\frac{\partial g}{\partial z}\right]\ .\end{aligned} \tag{2.23}$$

ξ is the canonical conjugate variable of z. In the rest of this work, unless otherwise stated, it is understood that the independent arguments of the functions are z and ξ. The complex manifold $\mathcal{M}$ is a coset space for the groups and is a sphere for SU(2), a hyperboloid for SU(1,1), and a plane for W_1. The parameter α defined in (2.16) is then interpreted as the curvature of the corresponding manifold. For the simple cases treated here this manifold has dimension two and corresponds to the phase space of a

system with one degree of freedom. For other groups the dimensionality is in general that of the orbits under the coadjoint action of the group.[8]

The Laplace-Beltrami operator on $\mathcal{M}$ is given by

$$\Delta=\left[\frac{\partial^2 F}{\partial z\partial\bar{z}}\right]^{-1}\frac{\partial^2}{\partial z\partial\bar{z}}=(1+\alpha z\bar{z})^2\frac{\partial^2}{\partial z\partial\bar{z}}\ . \tag{2.24}$$

Alternatively, in terms of the variable z,ξ

$$\Delta=\frac{\partial}{\partial\xi}\left[\frac{\partial}{\partial z}-\alpha\xi^2\frac{\partial}{\partial\xi}\right]\ . \tag{2.25}$$

These geometrical structures determine the manifold $\mathcal{M}$ as a phase space (though in general with a more complicated structure than the usual classical phase space of mechanical systems).

The set of coherent states constitutes also an overcomplete basis for the representation of each group. This can be symbolized in a resolution of unity

$$I=\int d\mu(z)\frac{|z\rangle\langle z|}{\langle z|z\rangle} \tag{2.26}$$

where the measure is

$$d\mu(z)=\frac{\lambda}{\pi}\frac{\partial^2 F}{\partial z\partial\bar{z}}d(\mathrm{Re}z)d(\mathrm{Im}z)\ . \tag{2.27}$$

The action of operators on $\mathcal{M}$ can be represented in the following two ways. As integral kernels using (2.26) any operator can be written as

$$\hat{A}=\int d\mu(z)d\mu(y)\langle z|\hat{A}|y\rangle\frac{|z\rangle\langle y|}{\langle z|z\rangle\langle y|y\rangle}\ . \tag{2.28}$$

However, the analyticity of the coherent states allows a simpler representation in terms of diagonal kernels as

$$\hat{A}=\int d\mu(z)\frac{|z\rangle\langle z|}{\langle z|z\rangle}A^0(z,\xi)\ . \tag{2.29}$$

Another representation is in terms of diagonal matrix elements

$$A(z,\xi)=\frac{\langle z|\hat{A}|z\rangle}{\langle z|z\rangle} \tag{2.30}$$

which is related to A^0 in (2.29) by

$$A(z,\xi)=\int d\mu(y)\frac{\langle z|y\rangle\langle y|z\rangle}{\langle y|y\rangle}A^0(y,\nu) \tag{2.31}$$

where $\nu=\bar{y}/(1+\alpha y\bar{y})$. Here, as stated previously, we are taking (z,ξ) and (y,ν) as independent variables. Both A and A^0 fully represent the quantum operators $\hat{A}$ and are known as covariant (or Q) symbol and contravariant (or P) symbol. They map the operator into a c-number function on the classical manifold $\mathcal{M}$. Their relationship has been extensively studied. For our purposes we are only interested in their *asymptotic* relationship (see Appendix D):

$$A=TA^0=(1+\Delta/\lambda+\cdots)A^0\ . \tag{2.32}$$

In (2.32) we have used the expansion parameter λ defined in (2.17).

Alternatively, a differential realization of the action of an operator can be obtained using (2.6), (2.10), or (2.15). Thus

$$\langle z|\hat{A}|\psi\rangle=\hat{A}\left[z,\frac{d}{dz}\right]\langle z|\psi\rangle\ . \tag{2.33}$$

We will always assume that the operator in (2.33) has been "normal" ordered with all operators d/dz acting on the right.

A relationship of $\hat{A}(z,d/dz)$ with the Q symbol is easily obtained from (2.33) as

$$A(z,\xi)=\frac{\langle z|\hat{A}|z\rangle}{\langle z|z\rangle}=\frac{1}{\langle z|z\rangle}\hat{A}\left[z,\frac{d}{dz}\right]\langle z|z\rangle\ . \tag{2.34}$$

In this representation the Schrödinger equation is

$$\hat{H}\left[z,\frac{d}{dz}\right]\langle z|\psi\rangle=E\langle z|\psi\rangle\ . \tag{2.35}$$

In the solution of this equation the requirement of analyticity is essential and provides the quantization of energy.[12]

III. ASYMPTOTIC EXPANSIONS

We turn now to the solution of the stationary Schrödinger equation (2.35) in the limit for large λ. *It is important to notice that we do the expansion in* $\lambda=\Omega+\alpha$ *and not, for example, directly in* Ω.

We first expand the Hamiltonian in normal form as

$$\hat{H}\left[z,\frac{d}{dz}\right]=\sum_m f_m(z,\lambda)\left[\frac{1}{\lambda}\frac{d}{dz}\right]^m\ . \tag{3.1}$$

The asymptotic expansion of (2.35) is obtained with the usual WKB-like ansatz

$$\langle z|\psi\rangle=\exp[\lambda S(z)]\ . \tag{3.2}$$

Substituting (3.2) in (2.35) and using the fact that

$$e^{-\lambda S}\frac{d}{dz}e^{\lambda S}=\lambda S'+\frac{d}{dz} \tag{3.3}$$

we get

$$\hat{H}(z,S'(z)+(1/\lambda)(d/dz))1=E \tag{3.4}$$

where primes indicate derivative with respect to z. The rather symbolic expression (3.4) can be expanded explicitly in terms of $1/\lambda$ as follows:

$$E=\left[\hat{H}(z,u)+\frac{1}{2!\lambda}S''(z)\frac{\partial^2}{\partial u^2}\hat{H}(z,u)+\frac{1}{3!\lambda^2}S'''(z)\frac{\partial^3}{\partial u^3}\hat{H}(z,u)+\cdots\right]\Bigg|_{u=S'(z)} \tag{3.5}$$

where $\hat{H}(z,u)$ is (3.1) replacing $(1/\lambda)(d/dz)$ by u. This equation is an exact nonlinear equation for S which is equivalent to (2.35). In Appendix A we rewrite this expression up to order $1/\lambda$ in terms of the Q symbol $H(z,\xi)$ and its derivatives with the result

$$E=\Bigg\{H(z,y)+\frac{1}{2\lambda}\left[\alpha\left[y^2\frac{\partial^2}{\partial y^2}+2y\frac{\partial}{\partial y}\right]H(z,y)+S''(z)\frac{\partial^2}{\partial y^2}H(z,y)\right]+O(\lambda^{-2})\Bigg\}\Bigg|_{y=S'(z)}. \tag{3.6}$$

In what follows we shall invoke analytical continuation in order to assume that y belongs to an annular domain that contains a branch of the trajectory $y=\xi$ (cf. Ref. 4 for details). The last term in the right-hand side of (3.6) can be written in terms of a total derivative

$$S''(z)\frac{\partial^2 H(z,y)}{\partial y^2}\Bigg|_{y=S'(z)}=\frac{d}{dz}\left[\frac{\partial H(z,y)}{\partial y}\Bigg|_{y=S'(z)}\right]-\frac{\partial H(z,y)}{\partial z\partial y}\Bigg|_{y=S'(z)} \tag{3.7}$$

and then (3.6) becomes

$$E=H(z,y)|_{y=S'(z)}-\frac{1}{2\lambda}\Delta H(z,y)\Bigg|_{y=S'(z)}+\frac{1}{2\lambda}\frac{d}{dz}\left[\frac{\partial H(z,y)}{\partial y}\Bigg|_{y=S'(z)}\right]+O(\lambda^{-2}) \tag{3.8}$$

where we have used (2.25) for the Laplace-Beltrami operator Δ. The neat feature of (3.8) is that the first-order terms have assembled to form a differential operator with a geometrical significance plus a total derivative. It is important to remark that this only happens because we have used λ instead of Ω as an expansion parameter.

Equation (3.8) is solved order by order with

$$S=S_0+\frac{1}{\lambda}S_1+\cdots \tag{3.9}$$

obtaining

$$E=H(z,y)|_{y=S_0'(z)}+\frac{1}{\lambda}\left[S_1'(z)\frac{\partial H(z,y)}{\partial y}\Bigg|_{y=S_0'(z)}-\tfrac{1}{2}\Delta H(z,y)|_{y=S_0'(z)}+\frac{1}{2}\frac{d}{dz}\left[\frac{\partial H(z,y)}{\partial y}\Bigg|_{y=S_0'(z)}\right]\right]. \tag{3.10}$$

This yields the two equations

$$E=H(z,y)|_{y=S_0'(z)}, \tag{3.11}$$

$$S_1'(z)=-\frac{1}{2}\frac{d}{dz}\left[\ln\frac{\partial H(z,y)}{\partial y}\Bigg|_{y=S_0'(z)}\right]+\frac{1}{2}\frac{\Delta H}{\partial H/\partial y}\Bigg|_{y=S_0'(z)}. \tag{3.12}$$

The first is the Hamilton-Jacobi equation for S_0' in terms of the Q symbol as a classical Hamiltonian, and (3.12) can be used to compute the $1/\lambda$ correction $S_1(z)$.

In general, $H(z,\xi)$, includes various orders in λ and therefore the separation [(3.11), (3.12)] order by order in λ is somewhat arbitrary. We can use this fact to extract a classical Hamiltonian in such a way as to leave in (3.12) only the total derivative, rendering it trivially integrable. We are thus led to define a new classical Hamiltonian $\mathcal{H}_c$:

$$H=\left[1+\frac{\Delta}{2\lambda}+\cdots\right]\mathcal{H}_c,\quad \mathcal{H}_c=\left[1-\frac{\Delta}{2\lambda}+\cdots\right]H \tag{3.13}$$

in terms of which Eqs. (3.11) and (3.12) take the form

$$E=\mathcal{H}_c(z,y)|_{y=S_0'(z)}, \tag{3.14}$$

$$S_1'(z)=-\frac{1}{2}\frac{d}{dz}\left[\ln\frac{\partial\mathcal{H}_c(z,y)}{\partial y}\Bigg|_{y=S_0'(z)}\right]. \tag{3.15}$$

In the case of the Weyl group we verify that $\mathcal{H}_c$ defined in (3.13) coincides to this order with the "classical" Weyl-Wigner symbol $\mathcal{H}$ which is connected with the Q symbol H through (see, for example, Ref. 15)

$$H=\exp(\Delta/2\lambda)\mathcal{H}\simeq(1+\Delta/2\lambda+\cdots)\mathcal{H}. \tag{3.16}$$

For the SU(2) and SU(1,1) groups Berezin[16] has introduced the generalization of the Weyl-Wigner symbol, defining the Weyl covariant $\mathcal{A}$ and Weyl contravariant $\mathcal{A}^0$ symbols of an operator $\hat{A}$. For our purposes we only need the asymptotic relation of $\mathcal{H}$ and $\mathcal{H}^0$ with the Q symbol, which in Appendix D are shown to be

$$H=(1+\Delta/2\lambda+\cdots)\mathcal{H}, \tag{3.17}$$

$$H=(1+\Delta/2\lambda+\cdots)\mathcal{H}^0. \tag{3.18}$$

We see that, up to this order, these symbols $\mathcal{H}$ and $\mathcal{H}^0$ coincide and both agree with the expression (3.13).

In any of the three groups, the simplest way to compute the wave function, correct up to second order in $1/\lambda$, is then to use a classical Hamiltonian satisfying the asymptotic relation (3.13)—so that $\mathcal{H}_c$ is "half way" between the Q and P symbols as results from the comparison of Eqs. (3.13) and (2.32). In that case, (3.14) and (3.15) are applicable, and the first-order correction for the energy is trivially computed, as will be done in Sec. IV.

Then from (3.14) and (3.15) the asymptotic solution to (2.35) now becomes

$$\langle z|\psi\rangle=\left[\frac{\partial\mathcal{H}_c(z,y)}{\partial y}\Bigg|_{y=S_0'(z)}\right]^{-1/2}\exp[\lambda S_0(z)] \tag{3.19}$$

where

$$S_0(z)=\int^z y(z',E)dz' \tag{3.20}$$

and $y(z,E)$ has been obtained inverting algebraically the equation $\mathcal{H}_c(z,y)=E$. This is a WKB-like solution which, however, has some characteristic differences

which are worthwhile to point out. The prefactor is analogous to the $1/\sqrt{p(q,E)}$ of the WKB theory. However, since we are now in phase space and there are no turning points on the classical trajectory, the prefactor does not diverge and (3.19) provides a regular approximation in a neighborhood of the trajectory.

IV. QUANTIZATION IMPOSED

The requirement of analyticity for $\langle z|\psi\rangle$ inside the trajectory imposes the quantization of energy. This fact can be used to derive quantization conditions similar in nature to the Bohr-Sommerfeld rules. Since

$$\frac{dS(z)}{dz}=\frac{1}{\langle z|\psi\rangle}\frac{d}{dz}\langle z|\psi\rangle \tag{4.1}$$

then, for finite λ, and for a circuit $\mathcal{C}$ in the complex plane in a neighborhood of a branch of the trajectory

$$\lambda\oint_{\mathcal{C}}S'(z)dz=i\lambda\Delta(\arg\langle z|\psi\rangle)=2\pi i n,\quad n=0,1,\ldots \tag{4.2}$$

where $\Delta[f]$ is the jump of f around $\mathcal{C}$ and n is the number of zeros of $\langle z|\psi\rangle$ inside $\mathcal{C}$. When $\lambda\to\infty$ the function $S'(z)$ has, in general, cuts and poles in the complex z plane. According to (3.9) we impose the quantization by requiring that

$$I_0+\frac{I_1}{\lambda}+\frac{I_2}{\lambda^2}+\cdots=\frac{n}{\lambda} \tag{4.3}$$

where we have defined

$$I_i=\frac{\Delta S_i(E)}{2\pi i}=\frac{1}{2\pi i}\oint_{\mathrm{tr}}\frac{dS_i}{dz}(z,E)dz \tag{4.4}$$

where tr denotes the fact that we have chosen a branch of the trajectory as integration contour.

The integrals (4.4) can be interpreted as a particular case of the contour integrals of the form

$$\int_{\mathrm{tr}}[f_1(z,\bar z)dz+f_2(z,\bar z)d\bar z] \tag{4.5}$$

with $f_2=0$, $f_1=f_1(z)$ in the two-dimensional space of independent variables $z,\bar z$.

For I_0 we can hence write

$$I_0=\frac{1}{2\pi i}\int_{\mathrm{tr}}\frac{dS_0}{dz}(z,E)dz$$
$$=\frac{1}{2\pi i}\int_{\mathrm{tr}}\frac{\bar z}{1+\alpha z\bar z}dz=\frac{1}{2\pi i}\int_{\mathrm{tr}}\frac{\partial F}{\partial z}dz \tag{4.6}$$

where the integrands in the first and second integrals only coincide on the trajectory.

Using Stokes' theorem for the right-hand side of (4.6) we get

$$I_0=-\frac{1}{2\pi i}\int_{\mathrm{tr}}\frac{\partial^2 F}{\partial z\partial\bar z}dz\times d\bar z=\frac{1}{4\pi}\int_{\mathrm{tr}}\omega \tag{4.7}$$

where ω is the area two form on the manifold $\mathcal{M}$ [cf. (2.22)], so that $\int_{\mathrm{tr}}\omega$ is the area enclosed by the trajectory of energy E on $\mathcal{M}$.

Let us now compute the next term I_1. Using (3.15) for S_1' we get

$$I_1=\frac{1}{2\pi i}\int_{\mathrm{tr}}\frac{dS_1}{dz}dz=-\frac{1}{4\pi i}\int_{\mathrm{tr}}d\left[\ln\frac{\partial\mathcal{H}_c}{\partial y}\bigg|_{y=S_0'(z)}\right] \tag{4.8}$$

using the fact that the integral is over a branch of the trajectory and expressing it in terms of the independent variables $z,\bar z$ as in (4.5) we have

$$I_1=-\frac{1}{4\pi i}\int_{\mathrm{tr}}d\left[\ln\frac{\partial\mathcal{H}_c}{\partial y}\bigg|_{y=\xi(z,\bar z)}\right]. \tag{4.9}$$

Let us define

$$\gamma=\frac{1}{2\pi i}\int_{\mathrm{tr}}d\left[\ln\frac{\partial\mathcal{H}_c}{\partial y}\bigg|_{y=\xi(z,\bar z)}\right] \tag{4.10}$$

so that to these first two orders, from (4.3), (4.7), and (4.10) the quantization condition becomes ($\mathcal{E}$ denotes area)

$$\mathcal{E}=\int_{\mathrm{tr}}\omega=\frac{4\pi}{\lambda}\left[n+\frac{\gamma}{2}\right]\quad n=0,1,\ldots. \tag{4.11}$$

This is the general quantization for an arbitrary Hamiltonian $\mathcal{H}_c$ to this order; γ has to be calculated in each case. The integral (4.9) is obviously that of a form that is closed wherever $\ln(\partial\mathcal{H}_c/\partial y)|_{y=\xi(z,\bar z)}$ is a nonsingular function of $z,\bar z$. If we assume that the integration contour can be broken down into circuits surrounding each singularity and we further assume that $\partial\mathcal{H}_c/\partial y|_{y=\xi(z,\bar z)}$ is itself nonsingular inside the trajectory (this is not the case, for example, with the Coulomb potential) then γ is completely determined by the local properties of $\mathcal{H}_c$ in a neighborhood of each stationary point. In Appendix C we analyze this in more detail. In the well-known case of the Weyl group with a Hamiltonian of the form

$$H=\frac{p^2}{2m}+V(x) \tag{4.12}$$

with $V(x)$ a smooth function, γ is shown in Appendix C to be one, as expected. However, this phase-space calculation of the Maslov index reduces to counting the number of stable minus of unstable stationary points encircled by the classical trajectory.

Even though similar to the usual Bohr-Sommerfeld expression in coherent-state representation,[20] this formula differs in (i) that it uses classical orbits as calculated with $\mathcal{H}_c$ and (ii) we use $2\Omega+\alpha$ instead of 2Ω as expansion parameter.

Let us exemplify this with a trivial example of an SU(2) Hamiltonian

$$\hat H=-\hat J_z \tag{4.13}$$

so that Q and P symbols read

$$H=j(1-2z\xi)=\frac{(\lambda-1)}{2}(1-2z\xi), \tag{4.14}$$

$$H^0=(j+1)(1-2z\xi)=\frac{(\lambda+1)}{3}(1-2z\xi), \tag{4.15}$$

and, correct to next-to-leading order

$$\mathcal{H}_c \simeq \mathcal{H} \simeq \mathcal{H}^0 \simeq (j+\tfrac{1}{2})(1-2z\xi) = \frac{\lambda}{2}(1-2z\xi) \ . \tag{4.16}$$

The γ index is calculated easily (see Appendix C) to be

$$\gamma = 1 \ . \tag{4.17}$$

The classical trajectory is obtained from (4.16) by

$$\xi(z,E) = \left[1-\frac{2E}{\lambda}\right]\frac{1}{2z} \tag{4.18}$$

so that the quantization condition reads

$$\int_{\text{tr}} \omega = 2\pi\left[1-\frac{2E}{\lambda}\right] = \frac{4\pi}{\lambda}(n+\tfrac{1}{2}), \quad n=0,1,\ldots,\lambda-1 \tag{4.19}$$

or

$$E = \frac{\lambda}{2} - n - \tfrac{1}{2} = j-n, \quad n=0,1,\ldots,2j \tag{4.20}$$

which is the exact result.

This example was treated by Kuratsuji and Mizobuchi[20] in their study of the semiclassical approximation in the coherent-state representation for the spin group using the Q symbol for $\hat{H}$ and the same γ index, obtaining a result incorrect to next-to-leading order in λ (or in j). Notice the essential role played by the choice of the "classical" Hamiltonian and by the choice of expansion parameter λ (a fact already conjectured by them).

There are many other situations where one attempts to use the Q symbol as a classical Hamiltonian, the most notable being the time-dependent Hartree-Fock method. Although there is no expansion parameter there, the question of which is the most appropriate classical Hamiltonian, in the sense discussed in this paper, remains to be explored.

In this section we have found an approximation scheme for the energies by expanding the "action" [cf. (4.3) and (4.4)] in powers of $1/\lambda$ and imposing, for each order, a quantization condition (4.2).

A different strategy, often connected with perturbative corrections based on bosonizations,[21,22] is to expand the energy of the nth level $E(\lambda,n)$ in powers of $1/\lambda$. The coefficients are consequently, in general, n dependent.

In Appendix B we study the relation between both approaches. In particular, we show that Bohr-Sommerfeld approximation (without the γ index) is equivalent to a leading order in $1/\lambda$ but keeping $\beta \equiv n/\lambda$ as an independent parameter (i.e., a resummation of all terms in the expansion for the energies of the form n^α/λ^α).

V. HUSIMI DISTRIBUTION

In the large λ limit quantum dynamics reduces to a classical theory on the manifold $\mathcal{M}$ with the dynamics given by Hamilton's equations [cf. (2.23)]

$$\dot{z} = \{z,\mathcal{H}_c\} = i\left[\frac{\partial^2 F}{\partial z\,\partial\bar{z}}\right]^{-1}\frac{\partial \mathcal{H}_c}{\partial \bar{z}} \tag{5.1}$$

and the complex conjugate equation for $\bar{z}$.

We want to extract this behavior from our approximate expression for the wave function in the coherent-state representation. The square modulus of this wave function provides a positive phase-space distribution

$$W(z,\bar{z}) = \frac{|\langle z|\psi\rangle|^2}{\langle z|z\rangle} = \exp\left[\lambda\left[S+\bar{S}-\frac{1}{\lambda}\ln\langle z|z\rangle\right]\right] . \tag{5.2}$$

This is the Q symbol for the density operator. In the case of the Weyl group it is known as the Husimi distribution function.[18]

Using (3.9) and (2.18) for the norm, we can write to second order in λ

$$W(z,\bar{z}) = \exp\left[\lambda\left[A_0(x,\bar{z}) = \frac{1}{\lambda}A_1(z,\bar{z}) + \cdots\right]\right] \tag{5.3}$$

where

$$A_0(z,\bar{z}) = S_0(z) + \bar{S}_0(\bar{z}) - F(z,\bar{z}) \ , \tag{5.4}$$

$$A_1(z,\bar{z}) = S_1(z) + \bar{S}_1(\bar{z}) + \alpha F(z,\bar{z}) \ . \tag{5.5}$$

For large λ, $W(z,\bar{z})$ is sharply peaked at the point where $A_0(z,\bar{z})$ has a maximum:

$$\frac{\partial A_0}{\partial z} = \frac{\partial A_0}{\partial \bar{z}} = 0 \ . \tag{5.6}$$

Using (5.4) and (2.20) we see that this condition is satisfied by the points such that

$$\frac{\partial A_0(z,\bar{z})}{\partial z} = \frac{dS_0(z)}{dz} - \xi(z,\bar{z}) = 0 \tag{5.7}$$

(and simultaneously the complex conjugate equation). This is exactly the condition that determines S_0' as a solution to the Hamilton-Jacobi equation (3.14) and therefore the maxima occur on the classical trajectory.

To study the shape of the distribution close to the trajectory we expand $A_0(z,\bar{z})$ up to second order

$$\begin{aligned} A_0(z_c+\omega,\bar{z}_c+\bar{\omega}) = {} & A_0(z_c,\bar{z}_c) \\ & + \tfrac{1}{2}\left[\bar{\omega}^2\frac{\partial^2 A_0}{\partial \bar{z}^2} + 2\omega\bar{\omega}\frac{\partial^2 A_0}{\partial z\,\partial\bar{z}} \right. \\ & \left. + \omega^2\frac{\partial^2 A_0}{\partial z^2}\right] + \cdots \ , \end{aligned} \tag{5.8}$$

where the first derivatives vanish on account of (5.6) and the second derivatives are computed on the points $(z_c,\bar{z}_c)$ belonging to a classical trajectory of energy E. If the first term, which is a constant over the classical trajectory is included in the normalization, and using (5.7) it is easy to show that

$$A_0 = \frac{1}{2}\frac{\partial^2 F}{\partial z\,\partial\bar{z}}\left[\bar{\omega}^2\frac{dz}{d\bar{z}} - 2\omega\bar{\omega} + \omega^2\frac{d\bar{z}}{dz}\right] \tag{5.9}$$

where the derivatives are evaluated on $(z_c,\bar{z}_c)$.

Let us now define a unimodular complex number

$a^2 \equiv dz/d\bar{z}$ which clearly defines the direction of the trajectory. Then (5.8) becomes

$$A_0 = \frac{1}{2}\frac{\partial^2 F}{\partial z \partial \bar{z}}(\omega \bar{a} - \bar{\omega} a)^2 . \tag{5.10}$$

We notice that this form vanishes for ω in the direction of the trajectory [as was to be expected from (5.6)]. If we write the directions of ω relative to the trajectory using the real numbers ω_1, ω_2:

$$\omega_1 + i\omega_2 \equiv \omega \bar{a} \tag{5.11}$$

then

$$\omega = \omega_L + \omega_T \tag{5.12}$$

where we have defined the longitudinal and transversal components

$$\omega_L \equiv a\omega_1, \quad \omega_T \equiv ia\omega_2 . \tag{5.13}$$

Equation (5.10) then becomes

$$A_0 = -2\frac{\partial^2 F}{\partial z \partial \bar{z}}\omega_T \bar{\omega}_T = -\tfrac{1}{2}(\delta s_T)^2 \tag{5.14}$$

where δs_T is the length of ω_T [cf. (2.21)] using the local metric on $\mathcal{M}$.

Up to this order of approximation we can therefore write the distribution as

$$W(z,\bar{z}) = \exp\left[-\frac{\lambda}{2}(\delta s)^2\right] . \tag{5.15}$$

This is a Gaussian of constant height centered on the classical trajectory with a constant width $1/\sqrt{\lambda}$ where δs is the perpendicular distance from it measured with the metric on the manifold.

In order to find the factor that modulates the height we have to go to the next order A_1 in (5.3). According to this equation this will be a factor independent of λ but of course it will depend on the point on the trajectory.

Using (3.15) for S_1 and (5.3) we have (the formulas that follow should always be evaluated on the classical trajectory)

$$A_1(z,\bar{z}) = -\tfrac{1}{2}\ln\left|\frac{\partial \mathcal{H}_c}{\partial \xi}\right|^2 + \ln(1+\alpha z\bar{z}) . \tag{5.16}$$

Since

$$\frac{\partial \mathcal{H}_c(z,\xi)}{\partial \xi} = (1+\alpha z\bar{z})^2 \frac{\partial \mathcal{H}_c(z,\bar{z})}{\partial \bar{z}} \tag{5.17}$$

we have

$$\exp[A_1(z,\bar{z})] = \left[(1+\alpha z\bar{z})\left|\frac{\partial \mathcal{H}_c}{\partial c}\frac{\partial \mathcal{H}_c}{\partial \bar{z}}\right|^2\right]^{-1} . \tag{5.18}$$

We are putting $\mathcal{H}_c(z,\bar{z}) \equiv \mathcal{H}_c(z,\xi(z,\bar{z}))$. Since $W(z,\bar{z})$ gives the probability density on $\mathcal{M}$, we expect this factor to be inversely proportional to the phase-space velocity. Let us check that this is so. The velocity on $\mathcal{M}$ is given by [cf. (2.21)]

$$v = \frac{ds}{dt} = 2\left[\frac{\partial^2 F}{\partial z \partial \bar{z}}\dot{z}\,\dot{\bar{z}}\right]^{1/2} = \frac{2}{1+\alpha z\bar{z}}(\dot{z}\,\dot{\bar{z}})^{1/2} . \tag{5.19}$$

If we now use Hamilton's equations (5.1) for $\dot{z}$ and $\dot{\bar{z}}$ we get

$$v = 2(1+\alpha z\bar{z})\left|\frac{\partial \mathcal{H}_c}{\partial z}\frac{\partial \mathcal{H}_c}{\partial \bar{z}}\right|^{1/2} \tag{5.20}$$

and thus we see that, up to a normalization factor, (5.18) is the inverse of the phase-space velocity.

Finally, using these results, the large λ form of the Husimi distribution in the neighborhood of the point $(z_c, \bar{z}_c)$ on the trajectory can be written

$$W = \mathcal{N}\frac{1}{v(z_c,\bar{z}_c)}\exp\left[-\frac{\lambda}{2}(\delta s)^2\right] \tag{5.21}$$

where $\mathcal{N}$ is a constant normalization. An alternative and more useful expression can be written in terms of $\mathcal{H}_c(z,\bar{z})$:

$$W = \mathcal{N}\frac{1}{v(z,\bar{z})}\exp\left[-2\lambda\left|\frac{\mathcal{H}_c(z,\bar{z})-E}{v(z,\bar{z})}\right|^2\right] . \tag{5.22}$$

It is easy to check that this expression is the same as (5.21) close to the trajectory where its value is significant—E is the energy of the trajectory quantized by (4.11). Notice that the last two expressions are entirely written in terms of invariant geometric objects. It should be pointed out that the first-order correction only affects the height of the distribution function and not the locus of the maxima. Again this happens only due to the peculiar choice of classical Hamiltonian and expansion parameter.

The prefactor in (5.21) and (5.22) vanishes if the phase-space velocity is zero, as, for example, on an unstable stationary point on the trajectory when it coincides with a separatrix. This signals a breakdown of the approximations leading to Eq. (3.19) in the neighborhood of these points. However, the turning points (or caustics) that produce divergences in WKB in coordinate or momentum space are not present.

This result which is simple and intuitive should be compared to the equivalent calculation for the Wigner distribution as calculated by Berry[23] for the Weyl group. There the classical result gives a δ function on the trajectory, which, when broadened by a large but finite λ becomes an Airy-like function with very fast oscillation away from the trajectory to its concave side and a broad peak on it. In our case the δ function is broadened to a simple Gaussian on the phase-space manifold and the oscillations are eliminated.

VI. THE QUANTUM ROTOR

As an illustration of the results obtained in the preceding sections, we consider the dynamics of the asymmetric top

$$\hat{H} = \hat{J}_x^2 + \chi \hat{J}_y^2 - \hat{J}_z^2 \tag{6.1}$$

where we have used the standard parametrization.[24]

This is an example of an SU(2) Hamiltonian ($\alpha=1$). In the large j (or λ) limit the (classical) dynamics is represented by a constant modulus angular momentum vector describing a trajectory on the two-dimensional surface of the Bloch sphere.

Specific coherent states for this Hamiltonian have been considered by Janssen.[25] In our case we use the simpler SU(2) coherent states given by Eq. (2.8). We obtain for the Q and P symbol of Hamiltonian (6.1)

$$H(z,\xi)=(\lambda-1)(\lambda-2)\times[(\rho z^4+\sigma z^2+\rho)\xi^2-(2\rho z^3+\sigma z)\xi+\rho z^2-\tfrac{1}{4}]+\frac{(1-4\sigma)(\lambda-1)}{4}, \tag{6.2}$$

$$H^0(z,\xi)=(\lambda+1)(\lambda+2)\times[(\rho z^4+\sigma z^2+\rho)\xi^2-(2\rho z^3+\sigma z)\xi+\rho z^2-\tfrac{1}{4}]-\frac{(1-4\sigma)(\lambda+1)}{4} \tag{6.3}$$

where for this group $\lambda=2j+1$ and $\xi=\bar{z}/(1+z\bar{z})$. In (6.2) and (6.3) we have defined

$$\rho=\frac{1-\chi}{4},\quad \sigma=-\frac{3+\chi}{2}. \tag{6.4}$$

It is convenient to work with the scaled Hamiltonian

$$H\to H/\lambda^2 \tag{6.5}$$

so that H contains only terms up to order $1/\lambda^2$. Using Eq. (3.13) we calculate the classical symbol $\mathcal{H}_c$ as

$$\mathcal{H}_c\simeq\left[1-\frac{\Delta}{2\lambda}\right]H. \tag{6.6}$$

Up to order $1/\lambda$ we obtain

$$\mathcal{H}_c(z,\xi)=(\rho z^4+\sigma z^2+\rho)\xi^2-(2\rho z^3+\sigma z)\xi+\rho z^2-\tfrac{1}{4}+O(\lambda^{-2}), \tag{6.7}$$

i.e., the leading order term of Eqs. (6.2) and (6.3). Thus we see that the action of the operator $(1-\Delta/2\lambda)$ on H is to eliminate terms of order $1/\lambda$.

We are now in a position to apply the quantization condition (4.11). The classical Hamiltonian (6.7) obtained gives the usual dynamics for the angular momentum vector on the Bloch sphere with six stationary points corresponding to the three principal axes of inertia. Those associated with the major and minor axis are stable and the intermediate one is unstable. Each of them satisfies the equation $\partial\mathcal{H}_c(z,\xi)/\partial\xi=0$. Since every trajectory encircles one stable point, in order to determine the γ index we must calculate the integral (4.10) for a small contour around the stable point. Using standard techniques similar to those indicated in Appendix C, we obtain $\gamma=1$ and the quantization condition becomes

$$\int_{\rm tr}\omega=\int_0^{2\pi}[1+\cos\theta(\varphi,E)]d\varphi=\frac{4\pi}{2j+1}(n+\tfrac{1}{2}) \tag{6.8}$$

where $\int_{\rm tr}\omega$ is the area of the classical trajectory on the sphere and $\theta(\phi,E)$ is the parametrization of the trajectory of energy E using the spherical angles θ and ϕ. They are related to the coherent states coordinates by $z=\tan(\theta/2)e^{i\phi}$.

In this formula, since $\int_{\rm tr}\omega\le 4\pi$ we have

$$n\le 2j. \tag{6.9}$$

Notice that the change $n\to 2j-n$ amounts to quantizing using the complementary area on the sphere. The consistency of this condition requires that $2j$ be an integer, i.e., the quantization of j.

If we define

$$k=n-j,\quad k=-j,\ldots,j \tag{6.10}$$

then Eq. (6.8) reads

$$\int_0^{2\pi}\cos\theta\,d\varphi=\frac{4\pi k}{2j+1},\quad k=0,\pm1,\ldots,\pm j. \tag{6.11}$$

In his extensive study of the semiclassical quantization of the asymmetric rotor, King[24] has used empirically a similar quantization rule using the same Hamiltonian but rescaled by $j(j+1)$ instead of λ^2. His quantization condition is

$$\int_0^{2\pi}\cos\theta\,d\varphi=\frac{2\pi k}{\sqrt{j(j+1)}}. \tag{6.12}$$

Our results differ from theirs only at order $1/\lambda^2$ since we have

$$\lambda/[2\sqrt{j(j+1)}]=1+O(1/\lambda^2).$$

Thus we will not present a numerical comparison of energy levels and refer the reader to the work of King.

We have computed the wave functions and therefore we can present the Husimi distributions for the eigenstates. We have diagonalized the Hamiltonian (6.1) in a basis $|jm\rangle$ with $j=60$ and $\chi=-0.4$ corresponding to an oblate rotor. There are four subspaces characterized by the symmetry operations consisting in 180° rotations around the three axis. In Fig. 1 we present results for the $(+,+)$ block which has dimension $j/2+1=31$.

We plot the wave functions as distributions on the Bloch sphere. The normalization is arbitrary and has been chosen to enhance the graphical display. As expected from Eq. (5.21) the distributions peak neatly around the classical trajectories, which are obtained from the intersection of the Bloch sphere with the ellipsoid of inertia (Fig. 2). The oscillations in the height of the distributions are associated with variations in the classical velocity [cf. (5.21)]. The distribution peaks over the the two branches of the classical trajectory, a fact due to tunneling effects.

There are clearly three types of wave functions. From 1 to 10 the trajectories encircle the north and south poles and correspond to classical rotations with the angular momentum mostly aligned with the larger moment of inertia. States 11, 12, and 13 show the transition through the separatrix. It is interesting to notice the strong concentration of probability at the unstable point (state 12) corresponding to rotations around the intermediate axis. This is due to the fact that in that point the phase-space velocity is zero and thus there is a large probability of

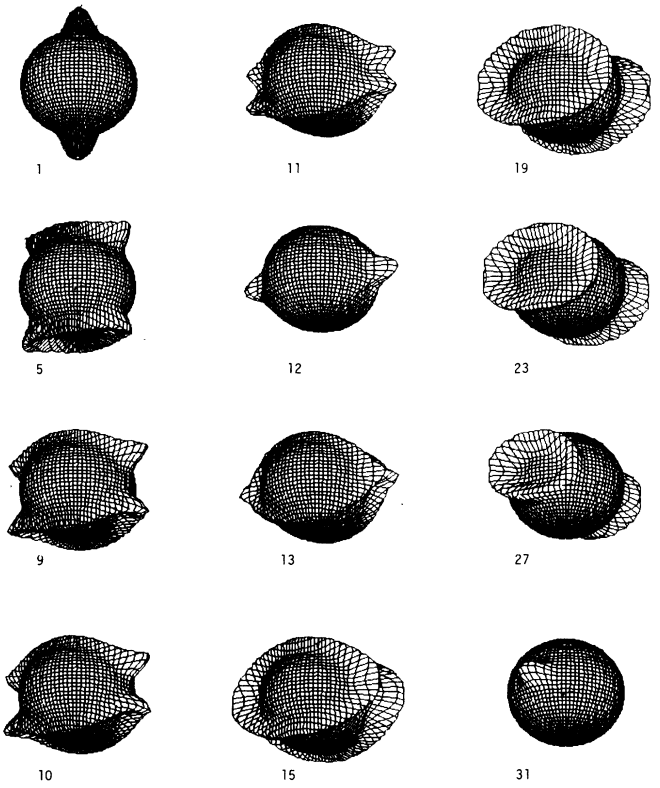

FIG. 1. Phase-space distributions corresponding to several eigenstates of the triaxial rigid rotor with $\chi=-0.4$ (see text).

finding a wave packet there. As discussed in Sec. V, our approximate expression would diverge for this point. If we continue increasing the energy (15–31), we get now distributions centered on trajectories that encircle the other two stable points, until we arrive at the eigenstate with higher energy, 31, that corresponds to a rotation around the axis with minimum moment of inertia.

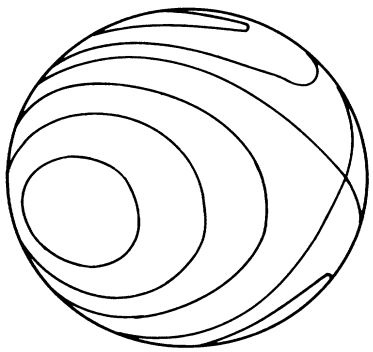

FIG. 2. Classical trajectories associated with the angular momentum vector on Bloch sphere for the triaxial rigid rotor with $\chi=-0.4$.

VII. CONCLUSIONS

We have discussed in detail the first two orders of the semiclassical expansion for the Weyl (W_1), SU(2), and SU(1,1) using the coherent-state representation. We have used analytic methods which closely parallel the standard WKB derivation but, by being in phase space, avoid the divergences associated with caustics.

By an appropriate definition of the classical Hamiltonian, which is neither the Q nor the P symbol, but something intermediate we are able to formulate a quantization rule correct to next-to-leading order in an asymptotic expansion in the parameter $1/\lambda$. The correction appears as a term of Maslov type related to the singular points of the Hamiltonian vector field enclosed by the classical trajectory. This is an intriguing relationship that deserves further study. Usually the Maslov index depends on the particular way a trajectory is inbedded in phase space. Here we have related it to whether the trajectory encircles a critical point of the Hamiltonian and therefore it is more like an index of its vector field. Whether this is a general property in more dimensions remains as an open question. Using this quantization rule one can get as a particular case for low excited states the excitation energies with perturbative corrections including anharmonicity effects.

The definition of the Hamiltonian coincides to this order with the Weyl-Wigner symbol of $\hat{H}$ for the W_1 group and with the Weyl-Berezin symbols for the SU(2) and SU(1,1) groups.

The square modulus of the semiclassical wave function provides a positive definite phase-space distribution. We show that this distribution peaks smoothly on the classical trajectories.

The generalization of our analytic methods to groups with more dimensions may seem at first sight trivial, but going to larger groups leads to phase spaces of dimension ≥ 2 where the systems are not in general integrable. In this case, although many of the techniques discussed in this paper can also be applied to the semiclassical limit, for analytical work one encounters very rapidly the same difficulties that appear for WKB in nonintegrable Hamiltonians. However, *as a representation method,* the phase-space positive distributions built from coherent states can be very useful for numerical work as they can be used to display wave functions in phase space and to allow a direct comparison with classical invariant structures.

ACKNOWLEDGMENTS

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APPENDIX A

In this appendix we derive Eq. (3.6). For convenience, we rewrite the differential operator representing the Hamiltonian (3.1) as

$$\hat{H}\left[z,\frac{1}{\lambda}\frac{d}{dz}\right]=\sum_m \frac{g_m(z)}{\gamma_m}\left[\frac{1}{\lambda}\frac{d}{dz}\right]^m \tag{A1}$$

where

$$\gamma_m=(\lambda-\alpha)(\lambda-2\alpha)\cdots(\lambda-m\alpha)\ . \tag{A2}$$

This expression defines $g_m(z)$.

We first calculate the Q symbol of the Hamiltonian defined by [cf. (2.34)]

$$H(z,\bar{z})=\frac{1}{\langle z|z\rangle}\hat{H}\left[z,\frac{d}{dz}\right]\langle z|z\rangle\ . \tag{A3}$$

For that purpose, let us show that

$$\frac{1}{\langle z|z'\rangle}\frac{d^m}{dz^m}\langle z|z'\rangle=\gamma_m\left[\frac{\bar{z}'}{1+\alpha z\bar{z}'}\right]^m \tag{A4}$$

with $\langle z|z'\rangle=(1+\alpha z\bar{z}')^{(\lambda-\alpha)/\alpha}$.

We proceed by induction, clearly, for $m=1$:

$$\frac{1}{\langle z|z'\rangle}\frac{d}{dz}\langle z|z'\rangle=(\lambda-\alpha)\frac{\bar{z}'}{1+\alpha z\bar{z}'}\ . \tag{A5}$$

If we assume that (A3) is valid for $m-1$, then for m

$$\begin{aligned}\frac{1}{\langle z|z'\rangle}\frac{d^m}{dz^m}\langle z|z'\rangle&=\frac{1}{\langle z|z'\rangle}\frac{d}{dz}\left[\frac{\langle z|z'\rangle}{\langle z|z'\rangle}\frac{d^{m-1}}{dz^{m-1}}\langle z|z'\rangle\right]\\&=\gamma_{m-1}(\lambda-m\alpha)\left[\frac{\bar{z}'}{1+\alpha z\bar{z}'}\right]^m\\&=\gamma_m\left[\frac{\bar{z}'}{1+\alpha z\bar{z}'}\right]^m\end{aligned} \tag{A6}$$

so that the Q symbol for H reads, using the variable ξ introduced in (2.20)

$$H(z,\xi)=\sum_m \frac{g_m(z)}{\lambda^m}\xi^m\ . \tag{A7}$$

Of course, the purpose of the inclusion of γ_m in (A1) was to eliminate it from (A6). Using (A1), Eq. (3.5) can be written, up to $1/\lambda$ terms

$$\sum_m \frac{g_m(z)}{\gamma_m}(S')^m+\frac{S''}{2\lambda}\sum_m \frac{g_m(z)}{\gamma_m}m(m-1)(S')^{m-2}=E \tag{A8}$$

but, γ_m can be approximated by

$$\frac{1}{\gamma_m}=\frac{1}{\lambda^m}+\frac{\alpha}{2\lambda^{m+1}}m(m+1)+\cdots \tag{A9}$$

so that, to that order

$$\sum_m \frac{g_m(z)}{\lambda^m}(S')^m+\frac{1}{\lambda}\left[\frac{\alpha}{2}\sum_m m(m+1)\frac{g_m(z)}{\lambda^m}(S')^m+\frac{S''}{2}\sum_m \frac{g_m(z)}{\gamma^m}m(m-1)(S')^{m-2}\right]+\cdots=E\ . \tag{A10}$$

According to definition (A7), the last equation can be expressed in terms of $H(z,\xi)$ as

$$\left[H(z,y)+\frac{1}{\lambda}\left[\frac{S''}{2}\frac{\partial^2}{\partial y^2}H(z,y)+\alpha y\frac{\partial H(z,y)}{\partial y}+\frac{\alpha y^2}{2}\frac{\partial^2}{\partial y^2}H(z,y)\right]\right]\Bigg|_{y=S'(z)}=E\ , \tag{A11}$$

i.e., Eq. (3.6).

APPENDIX B

In this appendix we study the relation between expressions for the energies based on expansions "in the action" of Secs. III and IV and the ordinary expansions of the energies in $1/\lambda$.

As indicated in Sec. IV the energies are obtained from

$$\frac{1}{2\pi i}\Delta S(\lambda,E)=\frac{n}{\lambda} \tag{B1}$$

or, using definition (4.3) and (4.4)

$$I(\lambda,E)=I_0(E)+\frac{1}{\lambda}I_1(E)+\cdots=\frac{n}{\lambda}\ . \tag{B2}$$

We consider now $\beta\equiv n/\lambda$ as an independent parameter so that inverting (B2) we get

$$E(\beta,\lambda)=I^{-1}(\beta,\lambda)\ . \tag{B3}$$

Let us formally expand (B3)

$$E(\beta,\lambda)=\sum_m \frac{E_m(\beta)}{\lambda^m}\ . \tag{B4}$$

To relate this expression to the usual expansions of the energy, we write (notice that this is not always possible, e.g., Coulomb potential)

$$E_m(\beta)=\sum_r d_r^m\beta^r \tag{B5}$$

so that

$$\begin{aligned}E(n,\lambda)&=\sum_{s\ (>r)} c_r^s\frac{n^r}{\lambda^s}\\&=c_0^0+\frac{c_1^1n+c_0^1}{\lambda}+\frac{c_2^2n^2+c_1^2n+c_0^2}{\lambda^2}+\cdots\end{aligned} \tag{B6}$$

where $c_r^s\equiv d_r^{s-r}$.

We next consider (B2) and substitute expression (B4) for the energy

$$I_0\left[E_0(\beta)+\frac{1}{\lambda}E_1(\beta)+\cdots\right]+\frac{1}{\lambda}I_1\left[E_0(\beta)+\frac{1}{\lambda}E_1(\beta)+\cdots\right]+\cdots=\beta \tag{B7}$$

where the large parentheses indicate the argument of the functions I_i. To the first two orders this equation reads

$$I_0(E_0)=\beta\ , \tag{B8a}$$

$$E_1\frac{\partial I_0}{\partial E}(E_0)+I_1(E_0)=0\ . \tag{B8b}$$

Comparing with (B6) we find that (B8a), i.e., the Bohr-Sommerfeld approximation, is equivalent to the summation of the principal series of (B6):

$$E_0(\beta)=c_0^0+c_1^1\beta+c_2^2\beta^2+\cdots=\sum_n c_n^n\beta^n \tag{B9}$$

so that we find that this approximation is the leading order of an expansion in powers of $1/\lambda$ but considering $\beta\equiv n/\lambda$ as an independent parameter.

In particular, we have

$$c_0^0=E_0(\beta=0)=I_0^{-1}(\beta=0)\ , \tag{B10}$$

$$c_1^1=\left.\frac{dE_0}{d\beta}\right|_{\beta=0}\ , \tag{B11}$$

$$c_2^2=\left.\frac{1}{2}\frac{d^2E_0}{d\beta^2}\right|_{\beta=0}\ , \tag{B12}$$

and also,

$$c_0^1=E_1|_{\beta=0}\ , \tag{B13}$$

$$c_2^1=\left.\frac{dE_1}{d\beta}\right|_{\beta=0}\ . \tag{B14}$$

If we now differentiate (B8a) we find that

$$\frac{\partial I_0}{\partial E_0}\frac{dE_0}{d\beta}=1 \tag{B15}$$

so that

$$c_1^1\left.\frac{dE_0}{d\beta}\right|_{\beta=0}=\left[\left.\frac{\partial I_0}{\partial E_0}\right|_{\beta=0}\right]^{-1}\equiv\omega|_{\beta=0}\ . \tag{B16}$$

The last equality defines the classical frequency. Differentiating (B8a) twice we obtain

$$\begin{aligned}c_2^2&=\left.\frac{1}{2}\frac{d^2E_0}{d\beta^2}\right|_{\beta=0}\\&=\left.\frac{1}{2}\frac{d\omega(\beta)}{d\beta}\right|_{\beta=0}=\left.\frac{1}{2}\frac{d\omega(E_0)}{dE_0}\frac{dE_0}{d\beta}\right|_{\beta=0}\\&=\left.\frac{1}{2}\left[\omega\frac{d\omega}{dE_0}\right]\right|_{\beta=0}\ .\end{aligned} \tag{B17}$$

Using Eq. (B8b) and the result of Sec. IV for I_1 we have

$$c_0^1=E_1(\beta=0)=-\frac{I_1}{\partial I_0/\partial E_0|_{\beta=0}}=\frac{\gamma}{2}\omega|_{\beta=0}\ , \tag{B18}$$

$$c_1^2=\left.\frac{dE_1}{d\beta}\right|_{\beta=0}=\left.\frac{\gamma}{2}\frac{d\omega}{d\beta}\right|_{\beta=0}=\left.\frac{\gamma}{2}\left[\omega\frac{d\omega}{dE_0}\right]\right|_{\beta=0}\ . \tag{B19}$$

Finally, we have, for the perturbed energy of the nth level relative to the ground state (notice that we are assuming that the lowest energy is for $n=0$),

$$\begin{aligned}E_n-E_{\text{ground state}}&=\left.\frac{1}{\lambda}n\omega\right|_{\beta=0}\\&\quad+\frac{1}{2\lambda^2}(n^2+\gamma n)\left.\left[\omega\frac{d\omega}{dE_0}\right]\right|_{\beta=0}\ .\end{aligned} \tag{B20}$$

The first term gives the usual harmonic spacing near the ground state, related to the classical frequency ω. It is usually calculated in many-body theories with the random-phase approximation. The second term contains a $1/\lambda$ correction to the spacing and an anharmonicity proportional to n^2. These corrections are usually obtained with special perturbative expansions, i.e., the nuclear field theory[21] or Holstein-Primakoff[22] bosonization.

APPENDIX C

In this appendix we give some useful formulas for the calculation of the index γ. It is a winding number and therefore a topological invariant. It does not depend on the energy as long as no singularities of the Hamiltonian vector field are crossed. We show that its value is determined by the critical points enclosed by the trajectory.

We assume that the integration circuit can be changed by varying the energy and reduced to a sum over small circuits at different energies $\gamma=\sum_j\gamma_j$, where

$$\gamma_j=\frac{1}{2\pi i}\oint_{\mathcal{C}(z_j,\xi_j)}d\left[\ln\left[\left.\frac{\partial\mathcal{H}_c}{\partial y}\right|_{y=\xi(z,\bar z)}\right]\right]\ . \tag{C1}$$

The point $(z_j,\xi_j)\equiv(z_j,\bar zj)$ is a stationary point (or a singularity of the gradient) of H and $\mathcal{C}$ is a contour which we parametrize in the following way:

$$z=z_j+\rho e^{i\phi}\ , \tag{C2}$$

$$\bar z=\bar z_j+\rho e^{-i\phi} \tag{C3}$$

where we will later let $\rho\to0$. The integral (C1) becomes, with this substitution, an ordinary integral in ϕ between $\phi=0$ and $\phi=2\pi$.

Applying the standard method for these integrals we make the new change of variables

$$x=e^{i\phi},\quad\frac{1}{x}=e^{-i\phi} \tag{C4}$$

and we define

$$f(x,\rho)=\left.\frac{\partial\mathcal{H}_c(z,\xi)}{\partial\xi}\right|_{z=z_j+\rho x} \tag{C5}$$

obtaining

$$\gamma_j=\lim_{\rho\to0}\frac{1}{2\pi i}\int_{|x|=1}\frac{df(x,\rho)}{f(x,\rho)}dx=n-p \tag{C6}$$

where n and p are the numbers of zeros and poles of f inside the circle of unit radius, respectively.

As an example, let us derive γ_j for the case of the Weyl group and a Hamiltonian of quadratic kinetic energy of the form

$$\mathcal{H}_c(z,\bar z)=-\frac{\alpha}{2}(z-\bar z)^2+V(z+\bar z) \tag{C7}$$

so that

$$\frac{\partial \mathcal{H}_c(z,\bar{z})}{\partial \bar{z}} = \alpha(z-\bar{z}) + \frac{\partial V(z+\bar{z})}{\partial \bar{z}} \tag{C8}$$

where V is assumed to be an analytic function of $z+\bar{z}$. Clearly, the extrema lie on the real axis. In the neighborhood of one minimum $\mathcal{H}_c$ can be written

$$\mathcal{H}_c(z,\bar{z}) \cong -\frac{\alpha}{2}(z-\bar{z})^2 + \frac{\beta}{2}(z+\bar{z})^2 + \sum_{n(>2)} \beta_n (z+\bar{z})^n \tag{C9}$$

so that $f(x,\rho)$ takes the form

$$f(x,\rho) = \alpha\rho\left[x-\frac{1}{x}\right] + \beta\rho\left[x+\frac{1}{x}\right] + \sum_{n(>2)} n\beta_n \rho^{n-1}\left[x+\frac{1}{x}\right]^{n-1} . \tag{C10}$$

If we assume that the local frequency $\beta \neq 0$, then keeping only the first two terms (linear in ρ) $f(x,\rho)$ has a pole in $x=0$ and zeros in $x_\pm = \pm\sqrt{(\alpha-\beta)/(\alpha+\beta)}$ which lie inside the unit circle if $\beta/\alpha > 0$ (stable minimum) and outside if $\beta/\alpha < 0$ (unstable extremum) so that for these cases

$$\gamma_i = \begin{cases} 1 & \text{stable point } (\beta/\alpha > 0) \\ -1 & \text{unstable point } (\beta/\alpha < 0) . \end{cases} \tag{C11}$$

In the case where $\beta = 0$ we must keep the first nonzero term in the potential

$$f(x,\rho) = \alpha\rho\left[x-\frac{1}{x}\right] + n\beta_n\rho^{n-1}\left[x+\frac{1}{x}\right]^{n-1} = \frac{\alpha\rho x^{n-2}(x^2-1) + n\beta_n\rho^{n-1}(1+x^2)^{n-1}}{x^{n-1}} . \tag{C12}$$

It is easy to see that for $\rho \to 0$ we will have $n-2$ zeros near $x=0$, $n-1$ poles in $x=0$ and the two zeros near $x_\pm = \pm 1$. For small but nonzero values of ρ the effect of the potential is to shift the zeros $x_\pm$ either inside or outside the circle $|x|=1$.

Putting

$$x_\pm = \pm 1 + v_\pm \tag{C13}$$

with $v_\pm$ infinitesimal so that

$$|x_\pm|^2 \simeq 1 \pm 2v_\pm \tag{C14}$$

and inserting (C13) in (C12), we get

$$|x_\pm|^2 \simeq 1 - \frac{2^n \rho^{n-2}\beta_n}{\alpha}(\pm 1)^{n-2} \tag{C15}$$

which shows that

$$\gamma_j = \begin{cases} 1 & \text{stable point } (\beta_n/\alpha > 0,\ n \text{ even}) \\ 0 & \text{saddle point } (n \text{ odd}) \\ -1 & \text{unstable point } (\beta_n/\alpha < 0,\ n \text{ even}) . \end{cases} \tag{C16}$$

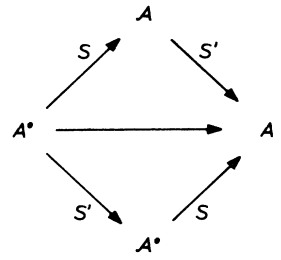
Clearly, from the above, for a particle in a potential of the form (C7), since always the number of stable points minus the number of unstable points is one, then

$$\gamma = \sum_j \gamma_j = 1 . \tag{C17}$$

Notice that in this derivation the quadratic form of the kinetic energy has played an essential role. In the general case, of course, γ need not be one.

APPENDIX D

Berezin[16] has defined generalizations of the Weyl-Wigner symbol of an operator $\hat{A}$: the Weyl covariant $\mathcal{A}$ and the Weyl contravariant $\mathcal{A}^0$ symbols. Their relation to the ordinary covariant A and contravariant A^0 Q and P symbols is as follows:



where $\mathcal{S}$, $\mathcal{S}'$, and T are functions of the Laplace-Beltrami operator.

We give a derivation of the asymptotic formulas for the operators T, $\mathcal{S}$ and $\mathcal{S}'$ in the SU(1,1) group. Similar results can be obtained for the SU(2) group, while the results for the Weyl group are well known.[15]

Recursion formulas for T, $\mathcal{S}$, and $\mathcal{S}'$ for this case are

$$T_\lambda = \left[1 - \frac{\Delta}{\lambda(\lambda+1)}\right]^{-1} T_{\lambda+1} , \tag{D1a}$$

$$\mathcal{S}_\lambda = \left[1 - \frac{\Delta}{\lambda(\lambda+1)}\right]^{-1} \mathcal{S}_{\lambda+2} , \tag{D1b}$$

$$\mathcal{S}'_\lambda = \left[1 - \frac{\Delta}{(\lambda+1)(\lambda+2)}\right]^{-1} \mathcal{S}'_{\lambda+2} . \tag{D1c}$$

Let us now assume that asymptotically

$$T_\lambda = 1 + \frac{\alpha_T}{\lambda} + \frac{\beta_T}{\lambda^2} + \cdots . \tag{D2}$$

Then, inserting expression (D2) in Eq. (D1a) and keeping only up to the second order

$$\left[1 + \frac{\alpha_T}{\lambda} + \frac{\beta_T}{\lambda^2} + \cdots\right]\left[1 - \frac{\Delta}{\lambda^2} + \cdots\right] = 1 + \frac{\alpha_T}{\lambda+1} + \frac{\beta_T}{(\lambda+1)^2} + \cdots . \tag{D3}$$

Expanding in powers of $1/\lambda$ and equating we find

$$T_\lambda = 1 + \frac{\Delta}{\lambda} + \cdots . \tag{D4}$$

Repeating the same procedure for $\mathcal{S}$ and $\mathcal{S}'$ we get

$$\mathcal{S}_\lambda = 1 + \frac{\Delta}{2\lambda} + \cdots , \tag{D5a}$$

$$\mathcal{S}'_\lambda = 1 + \frac{\Delta}{2\lambda} + \cdots , \tag{D5b}$$

and we verify that $\mathcal{S}\mathcal{S}' = T$ to this order. Equation (D4) was derived in Ref. 16 in a more rigorous way.

Applying the same method to the operators T, $\mathcal{S}$, and $\mathcal{S}'$ corresponding to the SU(2) group, we can check that formulas (D5a) and (D5b) are also valid for this group.

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