PHYSICAL REVIEW A VOLUME 49, NUMBER 5 MAY 1994

# Weyl-Wigner formalism for rotation-angle and angular-momentum variables in quantum mechanics

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(Received 7 July 1993)

A comprehensive study is presented on the Weyl-Wigner formalism for rotation-angle and angular-momentum variables: the elements of kinematics are extended, the elements of dynamics are established, and the implications of rotational perodicity and angular-momentum quantization are investigated. Particular attention is paid to discreteness, and two of its consequences are emphasized: the importance of evenness and oddness, and the need to use two difference operators in a discrete domain, whereas one differential operator suffices in a continuous domain. These consequences are shown to strongly distinguish the Weyl-Wigner formalism for rotation-angle and angular-momentum variables from the well-known Weyl-Wigner formalism for Cartesian-position and linear-momentum variables. The point is made clear that the first of these formalisms cannot be regarded as a trivial and straightforward extension of the second. The rotational Wigner function is derived as the only bilinear form of the state vector that is real, has the natural invariances for rotational motion, and yields the correct distributions for the rotation-angle and angular-momentum variables as well as the appropriate expression for the transition probability between states. The conditions for its uniqueness are thus established. Its properties are described in detail and, in particular, its uniform boundedness is demonstrated. The rotational Wigner function and the associated correspondence between quantum operators and classical-like functions, as well as the relations they obey, are explored and are written so as to clearly exhibit the distinct contributions of evenness and oddness in the discrete domain of the angular-momentum eigenvalues, thus providing a most natural way to account for periodicity. Using the derivative, which acts on the continuous rotation-angle variable, and the forward and backward differences, which act on the discrete angular-momentum variable, the equation of motion for the rotational Wigner function is established. This equation is detailed for the following Hamiltonian forms: those that depend only on the angular-momentum variable, including, in particular, the free rotator, and those that are in the cosine of the rotation-angle variable. It is verified that the Weyl-Wigner formalism for rotation-angle and angular-momentum variables has the correct nonperiodic limit and that it properly reduces to the Weyl-Wigner formalism for Cartesian-position and linear-momentum variables. In order to illustrate the formalism, a careful analysis is carried out for the rotational Wigner function representing the energy eigenstates of a hindered rotator whose Hamiltonian is the sum of a term in the absolute value of the angular-momentum variable with a term in the cosine of the rotation-angle variable. For this hindered rotator, and within the approximation of a large absolute value of the angular-momentum variable, the equation of motion for the rotational Wigner function is solved for its stationary solutions, and the time-independent Schrödinger equation is also solved.

PACS number(s): 03.65.Ca, 05.30.−d, 02.50.−r, 02.90.+p

## I. INTRODUCTION

The Weyl-Wigner formulation of nonrelativistic quantum mechanics using a classical-like phase-space language has been well established for variables such as the Cartesian position and linear momentum of a particle [1–3]. In this formalism, a correspondence exists between quantum operators and classical-like functions, the Weyl correspondence, and expectation values of dynamical variables are calculated as averages over a quasiprobability distribution, the Wigner function. For variables such as the rotation angle and angular momentum of a rotator, however, notorious difficulties arise due to periodicity [4]. Although the rotational Wigner function and associated correspondence between quantum operators and classical-like functions have already been introduced [5,6], the implications of rotational periodicity and angular-momentum quantization for the Weyl-Wigner formalism have not yet been fully analyzed. Kinematic properties such as natural invariances, uniqueness, and uniform boundedness of the rotational Wigner function remain to be investigated, as well as the particular features possessed by the formalism in the discrete domain of the angular-momentum eigenvalues. Moreover, and particularly important, the dynamics of the rotational Wigner function is still to be derived.

It is the purpose of the present article to provide a comprehensive and detailed study on the Weyl-Wigner formalism in the case of rotation-angle and angular-momentum variables. Notwithstanding the fact that the formalism has been extensively assessed in the case of

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Cartesian-position and linear-momentum variables, such a study is far from being a redundant exercise. In fact, as it becomes evident in this work, the results that apply to the former variables can by no means be regarded as a trivial and straightforward extension of those that apply to the latter. This does not come as a surprise, since the two types of variables are intrinsically different in quantum mechanics.

This article is organized as follows: the existing results on the Weyl-Wigner formalism are briefly reviewed in Sec. II, the kinematics of the rotational Wigner function and of the associated correspondence between quantum operators and classical-like functions is described and investigated in Sec. III, the dynamics of the rotational Wigner function is derived and discussed in Sec. IV, the Weyl-Wigner formalism is used to study a particular hindered rotator in Sec. V, and the results are summarized and conclusions are drawn in Sec. VI. For simplicity, only pure states and one rotational degree of freedom are considered.

## II. REVIEW OF THE FORMALISM

### A. Cartesian-position and linear-momentum variables

For completeness, and in order to better understand the differences encountered in the case of rotation-angle and angular-momentum variables, as well as to facilitate the comparison with the results to be derived in this work, it is useful to go briefly through the Weyl-Wigner formalism for Cartesian-position and linear-momentum variables. The results presented below can be found in the review works that have been published on the subject [1-3], as well as in the bibliography there provided. The Cartesian-position and linear-momentum operators $\hat{q}$ and $\hat{p}$, respectively, obey the well-known commutation and uncertainty relations, namely,

$$[\hat{q},\hat{p}]=i\hbar \ , \tag{2.1}$$

$$\Delta q(t)\Delta p(t)\geq\frac{\hbar}{2} \ , \tag{2.2}$$

and have continuous unbounded eigenvalues, represented by the variables $q$ and $p$,

$$\hat{q}|q\rangle=q|q\rangle \ , \quad \hat{p}|p\rangle=p|p\rangle \ . \tag{2.3}$$

Here $\hbar$ is the Planck constant divided by $2\pi$ and the fluctuation, at a given time $t$ and for a given pure state $|\psi(t)\rangle$, of the dynamical variable corresponding to the quantum operator $\hat{A}$ is defined, if $\hat{A}$ is Hermitian, as

$$\Delta A(t)=\{\langle[A(t)]^2\rangle-\langle A(t)\rangle^2\}^{1/2} \ , \tag{2.4}$$

with

$$\langle A(t)\rangle=\langle\psi(t)|\hat{A}|\psi(t)\rangle \ . \tag{2.5}$$

It is understood that the eigenvectors $|q\rangle$ and $|p\rangle$ form complete sets,

$$|\psi(t)\rangle=\int_{-\infty}^{+\infty}dq|q\rangle\langle q|\psi(t)\rangle=\int_{-\infty}^{+\infty}dp|p\rangle\langle p|\psi(t)\rangle \ , \tag{2.6}$$

and are normalized and related according to

$$\langle q|q'\rangle=\delta(q-q') \ , \quad \langle p|p'\rangle=\delta(p-p') \ , \quad \langle q|p\rangle=\frac{1}{(2\pi\hbar)^{1/2}}\exp(ipq/\hbar) \ , \tag{2.7}$$

and that $|\psi(t)\rangle$ is normalized to unity,

$$\langle\psi(t)|\psi(t)\rangle=\int_{-\infty}^{+\infty}dq|\langle q|\psi(t)\rangle|^2=\int_{-\infty}^{+\infty}dp|\langle p|\psi(t)\rangle|^2=1 \ . \tag{2.8}$$

The Wigner function representing $|\psi(t)\rangle$ is

$$W(p,q,t)=\frac{1}{\pi\hbar}\int_{-\infty}^{+\infty}dq'\exp(-i2pq'/\hbar)\langle q+q'|\psi(t)\rangle\times\langle\psi(t)|q-q'\rangle=\frac{1}{\pi\hbar}\int_{-\infty}^{+\infty}dp'\exp(-i2qp'/\hbar)\langle p-p'|\psi(t)\rangle\times\langle\psi(t)|p+p'\rangle \ . \tag{2.9}$$

This function is real and gives the correct distributions for $p$ and $q$,

$$\int_{-\infty}^{+\infty}dq\ W(p,q,t)=|\langle p|\psi(t)\rangle|^2 \tag{2.10}$$

and

$$\int_{-\infty}^{+\infty}dp\ W(p,q,t)=|\langle q|\psi(t)\rangle|^2 \ , \tag{2.11}$$

respectively. Therefore

$$\int_{-\infty}^{+\infty}dp\int_{-\infty}^{+\infty}dq\ W(p,q,t)=1 \ . \tag{2.12}$$

Moreover, the relation between $W(p,q,t)$ and $|\psi(t)\rangle$ is invariant with respect to translation, translational motion at constant linear velocity, position inversion, and time reversal. These invariances are the natural ones for translational motion, with the first two being the requirements for Galilean invariance. The function $W(p,q,t)$ in Eq. (2.9) may be uniquely defined as a bilinear form of $|\psi(t)\rangle$ that is real, possesses the above stated invariances, yields the proper distributions for the variables according to Eqs. (2.10) and (2.11), and is such that the transition probability between the states $|\psi(t)\rangle$ and $|\psi'(t)\rangle$ is given, in terms of the respective $W(p,q,t)$ and $W'(p,q,t)$, by

$$|\langle\psi(t)|\psi'(t)\rangle|^2=2\pi\hbar\int_{-\infty}^{+\infty}dp\int_{-\infty}^{+\infty}dq\ W(p,q,t)W'(p,q,t) \ . \tag{2.13}$$

Therefore these are the conditions for its uniqueness. Setting $|\psi'(t)\rangle$ equal to $|\psi(t)\rangle$ in Eq. (2.13), a necessary condition for $W(p,q,t)$ to represent a pure state is derived, which is

$$\int_{-\infty}^{+\infty} dp \int_{-\infty}^{+\infty} dq [W(p,q,t)]^2 = \frac{1}{2\pi\hbar} . \qquad (2.14)$$

It may also be seen from Eq. (2.13), choosing $|\psi(t)\rangle$ and $|\psi'(t)\rangle$ to be orthogonal, that $W(p,q,t)$ cannot be everywhere positive and so is not strictly a probability distribution but rather a quasiprobability distribution. Applying the Schwarz inequality to Eq. (2.9), it is possible to show that $W(p,q,t)$ is uniformly bounded according to

$$|W(p,q,t)| \leq \frac{1}{\pi\hbar} . \qquad (2.15)$$

With a given classical-like function $A(p,q)$ the Weyl correspondence associates the quantum operator

$$\begin{aligned}\hat{A} &= \frac{1}{\pi\hbar}\int_{-\infty}^{+\infty} dp \int_{-\infty}^{+\infty} dq \int_{-\infty}^{+\infty} dq' \exp(-i2pq'/\hbar) A(p,q) |q-q'\rangle\langle q+q'| \\ &= \frac{1}{\pi\hbar}\int_{-\infty}^{+\infty} dp \int_{-\infty}^{+\infty} dq \int_{-\infty}^{+\infty} dp' \exp(-i2qp'/\hbar) A(p,q) |p+p'\rangle\langle p-p'| . \end{aligned} \qquad (2.16)$$

Inversely, $A(p,q)$ can be written in terms of the matrix elements of $\hat{A}$ as

$$\begin{aligned} A(p,q) &= 2\int_{-\infty}^{+\infty} dq' \exp(-i2pq'/\hbar) \langle q+q'|\hat{A}|q-q'\rangle \\ &= 2\int_{-\infty}^{+\infty} dp' \exp(-i2qp'/\hbar) \langle p-p'|\hat{A}|p+p'\rangle . \end{aligned} \qquad (2.17)$$

The expectation value of the dynamical variable corresponding to $\hat{A}$ may then be expressed as an average of $A(p,q)$ over $W(p,q,t)$:

$$\begin{aligned} \langle A(t)\rangle &= \langle \psi(t)|\hat{A}|\psi(t)\rangle \\ &= \int_{-\infty}^{+\infty} dp \int_{-\infty}^{+\infty} dq\, A(p,q) W(p,q,t) . \end{aligned} \qquad (2.18)$$

It is important to note that there is a complete formal symmetry between $q$ and $p$, as it is evident from Eqs. (2.9), (2.16), and (2.17). Also, the classical function $A_{\text{cl}}(p,q)$ corresponding to $\hat{A}$ is not, in general, $A(p,q)$, but it can be derived from the latter by taking the classical limit $\hbar \to 0$. Namely,

$$A_{\text{cl}}(p,q) = \lim_{\hbar\to 0} A(p,q) . \qquad (2.19)$$

Let $\hat{H}$ be the quantum Hamiltonian operator and $|\psi(t)\rangle$ a solution of the time-dependent Schrödinger equation

$$i\hbar \frac{d}{dt}|\psi(t)\rangle = \hat{H}|\psi(t)\rangle . \qquad (2.20)$$

Then, the equation of motion for $W(p,q,t)$ reads [7]

$$\partial_t W(p,q,t) = \frac{2}{\hbar}\sin\left[\frac{\hbar}{2}(\partial_q^H \partial_p^W - \partial_p^H \partial_q^W)\right] H(p,q) W(p,q,t) , \qquad (2.21)$$

where $H(p,q)$ is the classical-like function associated with $\hat{H}$ by the Weyl correspondence, according to Eq. (2.17). The classical limit of Eq. (2.21) is the Liouville equation

$$\partial_t W_{\text{cl}}(p,q,t) = (\partial_q^H \partial_p^W - \partial_p^H \partial_q^W) H_{\text{cl}}(p,q) W_{\text{cl}}(p,q,t) , \qquad (2.22)$$

with $W_{\text{cl}}(p,q,t)$ being defined in a manner similar to Eq. (2.19). For the free particle with mass $M$, in which case

$$\hat{H} = \frac{\hat{p}^2}{2M} , \qquad (2.23)$$

Eq. (2.21) becomes

$$\partial_t W(p,q,t) = -\frac{p}{M}\partial_q W(p,q,t) \qquad (2.24)$$

and is identical to its classical counterpart. It is worth pointing out that the Wigner function representing an energy eigenstate corresponds to a stationary solution of Eq. (2.21), as can be easily verified from Eq. (2.9).

### B. Rotation-angle and angular-momentum variables

In the quantum mechanics of rotational motion, the use of a rotation-angle operator $\hat{\theta}$ leads to difficulties with the Hermiticity of the angular-momentum operator $\hat{l}$. This is due to the fact that the variable $\theta$, representing the continuous unbounded eigenvalues of $\hat{\theta}$, is not periodic [4]. In particular, relations similar to those of Eqs. (2.1) and (2.2) are incorrect and lead to nonsense when applied to $\hat{\theta}$ and $\hat{l}$. The use of an operator with eigenvalues equal to $\theta \bmod 2\pi$ is not satisfactory, because the variable representing these eigenvalues, although periodic, has $2\pi$-spaced discontinuities. Such difficulties are best circumvented by writing commutation and uncertainty relations using the operator $\exp(i\hat{\theta})$ instead of $\hat{\theta}$, since the eigenvalues of the former can be represented by a continuous periodic variable. Then,

$$[\hat{l}, \exp(i\hat{\theta})] = \hbar \exp(i\hat{\theta}) , \qquad (2.25)$$

$$\Delta l(t)\{1 - |\langle \exp[i\theta(t)]\rangle|^2\}^{1/2} \geq \frac{\hbar}{2}|\langle \exp[i\theta(t)]\rangle| . \qquad (2.26)$$

Another distinctive feature of rotational motion is the quantization of the unbounded eigenvalues of $\hat{l}$, which are discrete and of the form $m\hbar$, with $m$ an integer variable. In this way, the eigenvalue equations for $\exp(i\hat{\theta})$ and $\hat{l}$ are

$$\begin{aligned} \exp(i\hat{\theta})|\theta\rangle &= \exp(i\theta)|\theta\rangle , \\ \hat{l}|m\rangle &= m\hbar|m\rangle , \end{aligned} \qquad (2.27)$$

and the following relations apply for the eigenvectors $|\theta\rangle$ and $|m\rangle$ and the state $|\psi(t)\rangle$:

$$|\psi(t)\rangle=\int_{-\pi}^{+\pi}d\theta|\theta\rangle\langle\theta|\psi(t)\rangle=\sum_{m=-\infty}^{+\infty}|m\rangle\langle m|\psi(t)\rangle\ , \tag{2.28}$$

$$\langle\theta|\theta'\rangle=\sum_{n=-\infty}^{+\infty}\delta(\theta-\theta'-2\pi n)\ ,$$

$$\langle m|m'\rangle=\delta_{m,m'}\ ,$$

$$\langle\theta|m\rangle=\frac{1}{(2\pi)^{1/2}}\exp(im\theta)\ , \tag{2.29}$$

$$\langle\psi(t)|\psi(t)\rangle=\int_{-\pi}^{+\pi}d\theta|\langle\theta|\psi(t)\rangle|^2=\sum_{m=-\infty}^{+\infty}|\langle m|\psi(t)\rangle|^2=1\ . \tag{2.30}$$

Few results can be found on the Weyl-Wigner formalism for rotation-angle and angular-momentum variables. The rotational Wigner function has been introduced [5] by properly modifying $W(p,q,t)$ given in Eq. (2.9) so as to preserve the consistency of the kinematic relations obeyed by the latter and has been derived [6] by using operator algebra to set up a real function that is formally similar to $W(p,q,t)$ and yields the appropriate replacements for Eqs. (2.10) and (2.11). So, the rotational Wigner function, which is discrete in $m$ and has period $2\pi$ in $\theta$, reads

$$W_m(\theta,t)=\frac{1}{\pi}\int_{-\pi/2}^{+\pi/2}d\theta'\exp(-i2m\theta')\langle\theta+\theta'|\psi(t)\rangle\times\langle\psi(t)|\theta-\theta'\rangle\ . \tag{2.31}$$

It is real, gives the appropriate distributions for $m$ and $\theta$,

$$\int_{-\pi}^{+\pi}d\theta\, W_m(\theta,t)=|\langle m|\psi(t)\rangle|^2 \tag{2.32}$$

and

$$\sum_{m=-\infty}^{+\infty}W_m(\theta,t)=|\langle\theta|\psi(t)\rangle|^2\ , \tag{2.33}$$

respectively, and is normalized according to

$$\sum_{m=-\infty}^{+\infty}\int_{-\pi}^{+\pi}d\theta\, W_m(\theta,t)=1\ . \tag{2.34}$$

The form of $W_m(\theta,t)$ in Eq. (2.31) implies that the quantum operator $\hat{A}$ associated with a given classical-like function $A_m(\theta)$ must be [6,8]

$$\hat{A}=\frac{1}{\pi}\sum_{m=-\infty}^{+\infty}\int_{-\pi}^{+\pi}d\theta\int_{-\pi/2}^{+\pi/2}d\theta'\exp(-i2m\theta')A_m(\theta)|\theta-\theta'\rangle\langle\theta+\theta'|\ , \tag{2.35}$$

if the expectation value of the dynamical variable corresponding to $\hat{A}$ is to be written as

$$\langle A(t)\rangle=\langle\psi(t)|\hat{A}|\psi(t)\rangle=\sum_{m=-\infty}^{+\infty}\int_{-\pi}^{+\pi}d\theta\, A_m(\theta)W_m(\theta,t)\ . \tag{2.36}$$

A most instructive case, for which some results have already been obtained [5], is the hindered rotator whose Hamiltonian is

$$\hat{H}=\omega[|\hat{l}|-\gamma\cos(\hat{\theta})]\ , \tag{2.37}$$

with $\omega$ and $\gamma$ positive constants and

$$|\hat{l}||m\rangle=|m|\hbar|m\rangle\ . \tag{2.38}$$

Introducing in Eq. (2.31) the Wentzel-Kramers-Brillouin eigenfunction that represents, for the branch $m\gg1$, the energy eigenstate with energy

$$E_{m_0}\cong m_0\omega\hbar\ , \tag{2.39}$$

where $m_0\gg1$, the following expression results for the corresponding rotational Wigner function:

$$W_{m_0,m}(\theta)\cong\frac{1}{2\pi}J_{2(m-m_0)}\left[\frac{2\gamma}{\hbar}\cos(\theta)\right]+\frac{1}{\pi^2}\int_0^{\pi/2}d\phi\sin[2(m-m_0)\phi]\times\sin\left[\frac{2\gamma}{\hbar}\cos(\theta)\sin(\phi)\right]\ . \tag{2.40}$$

Here $J_\alpha(x)$ denotes the Bessel function of the first kind of order $\alpha$ and argument $x$. It is easy to show that the second term of Eq. (2.40) does not contribute to the distributions in $m$ and $\theta$ given by Eqs. (2.32) and (2.33). However, it is needed to ensure that $W_{m_0,m}(\theta)$ has the correct classical limit.

In pronounced contrast with the extensive work that has been devoted to the Weyl-Wigner formalism in $q$ and $p$, the existing elements on the Weyl-Wigner formalism in $\theta$ and $m$ are somewhat scarce and incomplete. Indeed, and as it becomes evident below, a detailed kinematic analysis remains to be carried out and no dynamic study has yet been performed. It is hoped, with the present article, to extend the ensemble of results on the Weyl-Wigner formulation of the quantum mechanics of rotational motion and, in particular, to explore the implications that discreteness, a major consequence of periodicity, has on the Weyl-Wigner formalism. In the following sections, the function $W_m(\theta,t)$ is derived from a set of natural requirements that uniquely determine its form, very much in the same way as $W(p,q,t)$ of Eq. (2.9) can be derived [3]. This approach is somewhat more satisfactory than the ones that have been proposed [5,6], in that $W_m(\theta,t)$ is constructed by proceeding from the conditions for its uniqueness and not by finding the appropriate formal replacements that allow to go from $W(p,q,t)$ to $W_m(\theta,t)$. Properties analogous to those of Eqs. (2.14) and (2.15) are established, and, in addition, $W_m(\theta,t)$ and the associated correspondence between $\hat{A}$ and $A_m(\theta)$ are thoroughly investigated in the discrete $m$ domain. Most important, the equation of motion for $W_m(\theta,t)$ is obtained. The nature of this equation is necessarily different from that of Eq. (2.21), since differential operators cannot be used in the $m$ domain. They are replaced here by difference operators, which are distinct in the following fundamental way: two operators must be used in a discrete domain, typically the forward and backward differences, whereas only one, the derivative, suffices in a continuous domain. It is also shown that the Weyl-Wigner formalism in $q$ and $p$ is a limiting case of the formalism in $\theta$ and $m$. So, as it has been mentioned in Sec. I, the second of these formalisms cannot stem from the first, a fact that does not prevent the existence of similarities between the two. To illustrate the features of the formalism here developed, an analysis is performed of the hindered rotator described by the Hamiltonian of Eq. (2.37).

## III. ELEMENTS OF KINEMATICS

### A. Derivation and uniqueness of the rotational Wigner function

The function $W_m(\theta,t)$ is derived here starting from a set of natural requirements that are shown to be the conditions for its uniqueness, which constitutes the most appropriate and straightforward way for constructing $W_m(\theta,t)$. In order to get familiarized with discreteness and its features, the eigenvectors $|m\rangle$ are used in the derivation, instead of $|\theta\rangle$. So, $W_m(\theta,t)$ is defined as a bilinear form of the state vector $|\psi(t)\rangle$,

$$W_m(\theta,t)=\langle\psi(t)|\hat{K}_m(\theta)|\psi(t)\rangle = \sum_{m'=-\infty}^{+\infty}\sum_{m''=-\infty}^{+\infty}\langle\psi(t)|m'\rangle\langle m'|\hat{K}_m(\theta)|m''\rangle \times\langle m''|\psi(t)\rangle \ , \tag{3.1}$$

that has the following properties: it is real,

$$\langle m'|\hat{K}_m(\theta)|m''\rangle=[\langle m''|\hat{K}_m(\theta)|m'\rangle]^* \ ; \tag{3.2}$$

it is invariant with respect to rotation,

$$\langle m'|\hat{K}_m(\theta)|m''\rangle=\exp[i(m'-m'')\phi] \times\langle m'|\hat{K}_m(\theta+\phi)|m''\rangle \ , \tag{3.3}$$

to rotational motion at constant angular velocity,

$$\langle m'|\hat{K}_m(\theta)|m''\rangle=\langle m'+n|\hat{K}_{m+n}(\theta)|m''+n\rangle \ , \tag{3.4}$$

to angle inversion,

$$\langle m'|\hat{K}_m(\theta)|m''\rangle=\langle -m'|\hat{K}_{-m}(-\theta)|-m''\rangle \ , \tag{3.5}$$

and to time reversal,

$$\langle m'|\hat{K}_m(\theta)|m''\rangle=[\langle -m'|\hat{K}_{-m}(\theta)|-m''\rangle]^* \ ; \tag{3.6}$$

it yields the correct probability distribution for $\theta$ according to Eq. (2.33),

$$\sum_{m=-\infty}^{+\infty}\langle m'|\hat{K}_m(\theta)|m''\rangle=\langle m'|\theta\rangle\langle\theta|m''\rangle =\frac{1}{2\pi}\exp[-i(m'-m'')\theta] \ ; \tag{3.7}$$

and it is such that the transition probability between the states $|\psi(t)\rangle$ and $|\psi'(t)\rangle$ is given, in terms of the respective $W_m(\theta,t)$ and $W'_m(\theta,t)$, by

$$|\langle\psi(t)|\psi'(t)\rangle|^2=2\pi\sum_{m=-\infty}^{+\infty}\int_{-\pi}^{+\pi}d\theta\, W_m(\theta,t)W'_m(\theta,t) \ . \tag{3.8}$$

Here Eqs. (3.3) and (3.4) must be valid for any $\phi$ and $n$, and Eq. (2.29) has been used in writing Eq. (3.7). These properties naturally replace those that apply in the case of $q$ and $p$ variables. In what follows, it is shown that Eqs. (3.1)–(3.8) suffice to determine the matrix elements $\langle m'|\hat{K}_m(\theta)|m''\rangle$ so that Eq. (3.1) turns out to be Eq. (2.31) for $W_m(\theta,t)$.

Replacing $\phi$ by $-\theta$ in Eq. (3.3) gives

$$\langle m'|\hat{K}_m(\theta)|m''\rangle =\exp[-i(m'-m'')\theta]\langle m'|\hat{K}_m(0)|m''\rangle \ . \tag{3.9}$$

Furthermore, from Eq. (3.4) it is inferred that, besides depending on $\theta$, $\langle m'|\hat{K}_m(\theta)|m''\rangle$ can depend only on $m-m'$ and $m-m''$ or, equivalently, on $2m-m'-m''$ and $m'-m''$. Therefore, Eq. (3.9) may be written as

$$\langle m'|\hat{K}_m(\theta)|m''\rangle =\exp[-i(m'-m'')\theta]K_{2m-m'-m'',m'-m''} \ , \tag{3.10}$$

with $K_{2m-m'-m'',m'-m''}$ such that

$$K_{2m-m'-m'',m'-m''}=(K_{2m-m'-m'',m'-m''})^* =K_{-2m+m'+m'',m'-m''} =K_{2m-m'-m'',-m'+m''} \ , \tag{3.11}$$

$$\sum_{m=-\infty}^{+\infty}K_{2m-m'-m'',m'-m''}=\frac{1}{2\pi} \ , \tag{3.12}$$

as follows from Eqs. (3.2) and (3.5)–(3.7). Next, using Eq. (3.8), which, taking into account Eqs. (3.1), (3.10), and (3.11), is equivalent to

$$|\langle\psi(t)|\psi'(t)\rangle|^2=(2\pi)^2\sum_{m=-\infty}^{+\infty}\sum_{n=-\infty}^{+\infty}\sum_{m'=-\infty}^{+\infty}\sum_{m''=-\infty}^{+\infty}K_{2m-m'-m'',m'-m''}K_{2(m-n)-m'-m'',m'-m''} \times\langle\psi(t)|m'\rangle\langle n+m'|\psi'(t)\rangle\langle\psi'(t)|n+m''\rangle\langle m''|\psi(t)\rangle \ , \tag{3.13}$$

it follows that

$$\sum_{m=-\infty}^{+\infty} K_{2m-m'-m'',m'-m''}K_{2(m-n)-m'-m'',m'-m''} = \frac{1}{(2\pi)^2}\delta_{n,0} . \quad (3.14)$$

At this point, it is convenient to perform the following transformation:

$$r=m-m'-m''+\Theta\left[\frac{m'+m''}{2}\right] ,$$
$$s=-m''+\Theta\left[\frac{m'+m''}{2}\right] , \quad (3.15)$$
$$\mu=m'+m''-2\Theta\left[\frac{m'+m''}{2}\right] ,$$

where $\Theta(x)$ denotes the largest integer not exceeding $x$ and $\mu$ is a binary variable that is either 0 or 1 and takes into account the evenness or oddness of $m'+m''$. It must be noted that $r$, $s$, and $\mu$ are independent variables and that, furthermore, Eq. (3.15) establishes a one-to-one correspondence between each pair $m'$ and $m''$ and each set $r$, $s$, and $\mu$ [9]. Henceforth, things become fundamentally different from the case of $q$ and $p$ variables and the particular features arising from discreteness become more and more evident, noticeably the importance of evenness and oddness. Through Eq. (3.15), $K_{2m-m'-m'',m'-m''}$ can be considered as a function of $r$, $s$, and $\mu$ and can thus be represented by

$$K_{2r+\mu,2s+\mu}=\frac{1}{2\pi}\int_{-\pi}^{+\pi}d\zeta\exp(ir\zeta)Q_{s,\mu}(\zeta) ,$$
$$Q_{s,\mu}(\zeta)=\sum_{r=-\infty}^{+\infty}\exp(-ir\zeta)K_{2r+\mu,2s+\mu} , \quad (3.16)$$

where $\zeta$ lies between $-\pi$ and $+\pi$ and $Q_{s,\mu}(\zeta)$ is a continuous function of $\zeta$ in this interval. This representation is particularly useful for solving Eq. (3.14), which is a convolution equation. Expressing Eqs. (3.11), (3.12), and (3.14) in terms of $\zeta$, $s$, and $\mu$ gives

$$Q_{s,\mu}(\zeta)=[Q_{s,\mu}(-\zeta)]^*=\exp(i\mu\zeta)Q_{s,\mu}(-\zeta) = Q_{-s-\mu,\mu}(\zeta) , \quad (3.17)$$

$$Q_{s,\mu}(0)=\frac{1}{2\pi} , \quad (3.18)$$

$$Q_{s,\mu}(\zeta)Q_{s,\mu}(-\zeta)=\frac{1}{(2\pi)^2} . \quad (3.19)$$

Therefore, from Eqs. (3.17) and (3.19),

$$[Q_{s,\mu}(\zeta)]^2=\frac{1}{(2\pi)^2}\exp(i\mu\zeta) , \quad (3.20)$$

and Eq. (3.18) implies that

$$Q_{s,\mu}(\zeta)=\frac{1}{2\pi}\exp\left[i\frac{\mu}{2}\zeta\right] . \quad (3.21)$$

Hence

$$K_{2r+\mu,2s+\mu}=\frac{1}{2\pi}\frac{\sin\left[\left[r+\frac{\mu}{2}\right]\pi\right]}{\left[r+\frac{\mu}{2}\right]\pi} . \quad (3.22)$$

So, combining Eqs. (3.15) and (3.22),

$$K_{2m-m'-m'',m'-m''} = \frac{1}{2\pi}\frac{\sin\left[\left[m-\frac{m'+m''}{2}\right]\pi\right]}{\left[m-\frac{m'+m''}{2}\right]\pi} = \frac{1}{(2\pi)^2}\int_{-\pi}^{+\pi}d\phi\exp\left[i\left[m-\frac{m'+m''}{2}\right]\phi\right] , \quad (3.23)$$

and then putting together Eqs. (3.1), (3.10), and (3.23), $W_m(\theta,t)$ reads

$$W_m(\theta,t)=\frac{1}{2\pi}\sum_{m'=-\infty}^{+\infty}\sum_{m''=-\infty}^{+\infty}\frac{\sin\left[\left[m-\frac{m'+m''}{2}\right]\pi\right]}{\left[m-\frac{m'+m''}{2}\right]\pi} \times\exp[i(m'-m'')\theta] \times\langle m'|\psi(t)\rangle\langle\psi(t)|m''\rangle , \quad (3.24)$$

which, considering Eqs. (2.28) and (2.29), is indeed equal to Eq. (2.31). Alternatively, $W_m(\theta,t)$ can be written as

$$W_m(\theta,t)=\frac{1}{2}\sum_{\mu=0,1}\sum_{m'=-\infty}^{+\infty}\frac{\sin\left[\left[m-m'-\frac{\mu}{2}\right]\pi\right]}{\left[m-m'-\frac{\mu}{2}\right]\pi}\times w_{m'+\mu/2}(\theta,t) = \frac{1}{2}w_m(\theta,t)+\frac{1}{2}\sum_{m'=-\infty}^{+\infty}\frac{(-1)^{m-m'-1}}{(m-m'-\frac{1}{2})\pi}\times w_{m'+1/2}(\theta,t) , \quad (3.25)$$

with

$$w_{m+\mu/2}(\theta,t)=\frac{1}{\pi}\sum_{m'=-\infty}^{+\infty}\exp\left[-i2\left[m'+\frac{\mu}{2}\right]\theta\right] \times\langle m-m'|\psi(t)\rangle \times\langle\psi(t)|m+m'+\mu\rangle = \frac{1}{\pi}\int_{-\pi}^{+\pi}d\theta'\exp\left[-i2\left[m+\frac{\mu}{2}\right]\theta'\right] \times\langle\theta+\theta'|\psi(t)\rangle\langle\psi(t)|\theta-\theta'\rangle . \quad (3.26)$$

Writing $W_m(\theta,t)$ as in Eqs. (3.25) and (3.26) is particularly suggestive, since the contributions of evenness and oddness, associated here with $w_m(\theta,t)$ and $w_{m+1/2}(\theta,t)$, respectively, appear clearly distinguished. The fact that these two contributions are quite different is an intrinsic feature of the Weyl-Wigner formalism in $\theta$ and $m$, which feature is to be encountered throughout the results established below. Besides, evenness and oddness are related to well-defined periodicities: $\pi$ for the former and $2\pi$ for the latter, as can be seen from Eq. (3.26). Accordingly, expressing $W_m(\theta,t)$ in terms of $w_{m+\mu/2}(\theta,t)$, as in Eq. (3.25), provides a most natural way to account for periodicity. The usefulness of working with $w_{m+\mu/2}(\theta,t)$, instead of $W_m(\theta,t)$ given by Eq. (2.31) or (3.24), is to be fully appreciated when studying the dynamics in Sec. IV.

### B. Properties of the rotational Wigner function

It is seen, from Eqs. (3.25) and (3.26), that $W_m(\theta,t)$ is not a straightforward discretization of the second of the forms given in Eq. (2.9) for $W(p,q,t)$ but is rather the result of a nontrivial summation of the real function $w_{m+\mu/2}(\theta,t)$. It is this function that does look like a discretization of that form, but a discretization performed so as to reflect the importance, conveyed by the variable $\mu$, of evenness and oddness in the discrete $m$ domain. It is also clear that $W_m(\theta,t)$ is unambiguously determined if $w_{m+\mu/2}(\theta,t)$ is known. Important properties of the latter, directly derived from Eq. (3.26), are

$$w_{m+\mu/2}(\theta+\pi,t)=(-1)^{\mu}w_{m+\mu/2}(\theta,t) , \tag{3.27}$$

$$\sum_{m=-\infty}^{+\infty} w_{m+\mu/2}(\theta,t)=|\langle\theta|\psi(t)\rangle|^2 +(-1)^{\mu}|\langle\theta+\pi|\psi(t)\rangle|^2 , \tag{3.28}$$

$$\int_{-\pi}^{+\pi}d\theta\, w_{m+\mu/2}(\theta,t)=2(1-\mu)|\langle m|\psi(t)\rangle|^2 , \tag{3.29}$$

$$\int_{-\pi}^{+\pi}d\theta\, w_m(\theta,t)w_{m'+1/2}(\theta,t)=0 . \tag{3.30}$$

It is worth mentioning the fact that $W_m(\theta,t)$ is not simply given in terms of $w_m(\theta,t)$. This can be understood with the help of Eq. (3.28), where it is shown that $w_m(\theta,t)$ cannot, in general, satisfy the normalization requirement imposed on $W_m(\theta,t)$ by Eq. (2.33) and hence the importance of $w_{m+1/2}(\theta,t)$ and of its contribution to $W_m(\theta,t)$. The actual relation between $W_m(\theta,t)$ and $w_m(\theta,t)$ can be derived from Eqs. (3.25) and (3.27) and is

$$W_m(\theta,t)+W_m(\theta+\pi,t)=w_m(\theta,t) . \tag{3.31}$$

Concerning Eq. (3.27), it provides a useful boundary condition when solving the equation of motion for $W_m(\theta,t)$, a point to be illustrated in Sec. V. Furthermore, Eq. (3.27) states that $w_m(\theta,t)$ and $w_{m+1/2}(\theta,t)$ do not have the same periodicity, a point already mentioned above, thus implying the orthogonality property of Eq. (3.30).

Before proceeding, it is convenient to write down two results that are of use in what follows. They are an immediate consequence of Eqs. (3.12), (3.14), and (3.23), and read

$$\sum_{m=-\infty}^{+\infty}\frac{\sin\left[\left[m-m'-\frac{\mu}{2}\right]\pi\right]}{\left[m-m'-\frac{\mu}{2}\right]\pi}=1 , \tag{3.32}$$

$$\sum_{m=-\infty}^{+\infty}\frac{\sin\left[\left[m-m'-\frac{\mu}{2}\right]\pi\right]}{\left[m-m'-\frac{\mu}{2}\right]\pi}\,\frac{\sin\left[\left[m-m''-\frac{\mu}{2}\right]\pi\right]}{\left[m-m''-\frac{\mu}{2}\right]\pi}=\delta_{m',m''} . \tag{3.33}$$

Following Eqs. (3.28) and (3.29), the probability distributions for $m$ and $\theta$ are given, in terms of $w_{m+\mu/2}(\theta,t)$ by

$$|\langle m|\psi(t)\rangle|^2=\tfrac{1}{2}\int_{-\infty}^{+\infty}d\theta\, w_m(\theta,t) \tag{3.34}$$

and

$$|\langle\theta|\psi(t)\rangle|^2=\tfrac{1}{2}\sum_{\mu=0,1}\sum_{m=-\infty}^{+\infty} w_{m+\mu/2}(\theta,t) , \tag{3.35}$$

respectively, and thus, recalling Eq. (2.30), the normalization condition

$$\tfrac{1}{2}\sum_{m=-\infty}^{+\infty}\int_{-\pi}^{+\pi}d\theta\, w_m(\theta,t)=1 \tag{3.36}$$

applies. It must be noted that $w_{m+1/2}(\theta,t)$ does not contribute to Eqs. (3.34) and (3.36). However, it does contribute to Eq. (3.35). The relations in Eqs. (3.34)–(3.36) are, of course, consistent with Eqs. (2.32)–(2.34), as it is easy to verify with the help of Eqs. (3.25), (3.29), and (3.32). They are to be recalled in Sec. V, in connection with the results quoted in Sec. II regarding the hindered rotator corresponding to Eq. (2.37).

Starting from Eq. (3.8), with $|\psi'(t)\rangle$ equal to $|\psi(t)\rangle$, and using Eqs. (3.25), (3.30), and (3.33), a necessary condition for $W_m(\theta,t)$ to represent a pure state can be established, which is of the same type as that of Eq. (2.14) and reads

$$\sum_{m=-\infty}^{+\infty}\int_{-\infty}^{+\infty}d\theta[W_m(\theta,t)]^2 =\tfrac{1}{4}\sum_{\mu=0,1}\sum_{m=-\infty}^{+\infty}\int_{-\pi}^{+\pi}d\theta[w_{m+\mu/2}(\theta,t)]^2=\frac{1}{2\pi} . \tag{3.37}$$

As it is to be shown in Sec. V, this condition may provide a useful test on the correctness of a particular $w_{m+\mu/2}(\theta,t)$. In the same manner as it has been done in connection with Eq. (2.13), Eq. (3.8) may be used to demonstrate that $W_m(\theta,t)$ cannot be everywhere positive.

A further property to be established here is the uniform boundedness of $W_m(\theta,t)$. From Eq. (3.25), it is immediate to see that

$$|W_m(\theta,t)| \le \tfrac{1}{2}\sum_{\mu=0,1}\left|\sum_{m'=-\infty}^{+\infty}\frac{\sin\left[\left(m-m'-\frac{\mu}{2}\right)\pi\right]}{\left(m-m'-\frac{\mu}{2}\right)\pi}w_{m'+\mu/2}(\theta,t)\right| . \tag{3.38}$$

Next, combining Eqs. (3.26) and (3.38), using the Cauchy inequality, and performing some straightforward algebra, it follows that

$$\left|\sum_{m'=-\infty}^{+\infty}\frac{\sin\left[\left(m-m'-\frac{\mu}{2}\right)\pi\right]}{\left(m-m'-\frac{\mu}{2}\right)\pi}w_{m'+\mu/2}(\theta,t)\right|^2$$
$$\le \frac{1}{\pi^2}\left|\sum_{m'=-\infty}^{+\infty}\frac{\sin\left[\left(m'+\frac{\mu}{2}\right)\pi\right]}{\left(m'+\frac{\mu}{2}\right)\pi}\exp\left[-i2\left(m'+\frac{\mu}{2}\right)\theta\right]\right|^2$$
$$\times\left[\sum_{m''=-\infty}^{+\infty}|\exp(i2m''\theta)\langle m''|\psi(t)\rangle|^2\right]\left[\sum_{m''=-\infty}^{+\infty}|\exp(-i2m\theta)\langle\psi(t)|m''\rangle|^2\right] , \tag{3.39}$$

which, considering Eq. (2.30), is equivalent to

$$\left|\sum_{m'=-\infty}^{+\infty}\frac{\sin\left[\left(m-m'-\frac{\mu}{2}\right)\pi\right]}{\left(m-m'-\frac{\mu}{2}\right)\pi}w_{m'+\mu/2}(\theta,t)\right| \le \frac{1}{\pi}\left|\sum_{m'=-\infty}^{+\infty}\frac{\sin\left[\left(m'+\frac{\mu}{2}\right)\pi\right]}{\left(m'+\frac{\mu}{2}\right)\pi}\exp\left[-i2\left(m'+\frac{\mu}{2}\right)\theta\right]\right| . \tag{3.40}$$

Now, recalling the equality in Eq. (3.23),

$$\left|\sum_{m'=-\infty}^{+\infty}\frac{\sin\left[\left(m'+\frac{\mu}{2}\right)\pi\right]}{\left(m'+\frac{\mu}{2}\right)\pi}\exp\left[-i2\left(m'+\frac{\mu}{2}\right)\theta\right]\right| = \left|\frac{1}{2\pi}\sum_{m'=-\infty}^{+\infty}\int_{-\pi}^{+\pi}d\phi\exp\left[i\left(m'+\frac{\mu}{2}\right)(\phi-2\theta)\right]\right|$$
$$=\left|\sum_{n=-\infty}^{+\infty}\int_{-\pi}^{+\pi}d\phi\exp\left[i\frac{\mu}{2}(\phi-2\theta)\right]\delta(\phi-2\theta-2\pi n)\right| = 1 . \tag{3.41}$$

Hence Eqs. (3.38), (3.40), and (3.41) yield

$$|W_m(\theta,t)| \le \frac{1}{\pi} , \tag{3.42}$$

which has a strong similarity with Eq. (2.15). It is instructive to see that Eq. (3.42) can also be established from Eq. (2.31), by applying the Schwarz inequality to the latter, recognizing that

$$\int_{-\pi/2}^{+\pi/2}d\theta'|\langle\theta+\theta'|\psi(t)\rangle|^2 \le \int_{-\pi}^{+\pi}d\theta'|\langle\theta+\theta'|\psi(t)\rangle|^2$$
$$=\int_{-\pi}^{+\pi}d\theta'|\langle\theta'|\psi(t)\rangle|^2 , \tag{3.43}$$

and then using Eq. (2.30). Another result, which can be derived by applying the Schwartz or the Cauchy inequality to Eq. (3.26), is

$$|w_{m+\mu/2}(\theta,t)| \le \frac{1}{\pi} . \tag{3.44}$$

### C. Correspondence between quantum operators and classical-like functions

Let the classical-like function associated with a given quantum operator $\hat{A}$ be

$$A_m(\theta)=2\int_{-\pi/2}^{+\pi/2}d\theta'\exp(-i2m\theta')\langle\theta+\theta'|\hat{A}|\theta-\theta'\rangle$$
$$=\sum_{m'=-\infty}^{+\infty}\sum_{m''=-\infty}^{+\infty}\frac{\sin\left[\left[m-\frac{m'+m''}{2}\right]\pi\right]}{\left[m-\frac{m'+m''}{2}\right]\pi}\times\exp[i(m'-m'')\theta]\langle m'|\hat{A}|m''\rangle \quad (3.45)$$

or, equivalently,

$$A_m(\theta)=\frac{1}{2}\sum_{\mu=0,1}\sum_{m'=-\infty}^{+\infty}\frac{\sin\left[\left[m-m'-\frac{\mu}{2}\right]\pi\right]}{\left[m-m'-\frac{\mu}{2}\right]\pi}a_{m'+\mu/2}(\theta), \quad (3.46)$$

with

$$a_{m+\mu/2}(\theta)=2\sum_{m'=-\infty}^{+\infty}\exp\left[-i2\left[m'+\frac{\mu}{2}\right]\theta\right]\times\langle m-m'|\hat{A}|m+m'+\mu\rangle$$
$$=2\int_{-\pi}^{+\pi}d\theta'\exp\left[-i2\left[m+\frac{\mu}{2}\right]\theta'\right]\times\langle\theta+\theta'|\hat{A}|\theta-\theta'\rangle . \quad (3.47)$$

Then, taking into account that

$$\sum_{m=-\infty}^{+\infty}\int_{-\pi}^{+\pi}d\theta\, A_m(\theta)W_m(\theta,t)$$
$$=\frac{1}{4}\sum_{\mu=0,1}\sum_{m=-\infty}^{+\infty}\int_{-\pi}^{+\pi}d\theta\, a_{m+\mu/2}(\theta)w_{m+\mu/2}(\theta,t) , \quad (3.48)$$

which can be derived in a manner analogous to Eq. (3.37), and that

$$\frac{1}{4}\sum_{\mu=0,1}\sum_{m=-\infty}^{+\infty}\int_{-\pi}^{+\pi}d\theta\, a_{m+\mu/2}(\theta)w_{m+\mu/2}(\theta,t)$$
$$=\langle\psi(t)|\hat{A}|\psi(t)\rangle , \quad (3.49)$$

which follows from Eqs. (3.26) and (3.47), it is easy to see that Eq. (2.36) is indeed verified. An alternative expression for the expectation value of the dynamical variable corresponding to $\hat{A}$ is then

$$\langle A(t)\rangle=\frac{1}{4}\sum_{\mu=0,1}\sum_{m=-\infty}^{+\infty}\int_{-\pi}^{+\pi}d\theta\, a_{m+\mu/2}(\theta)w_{m+\mu/2}(\theta,t) . \quad (3.50)$$

Inversely, $\hat{A}$ is written in terms of $A_m(\theta)$ according to Eq. (2.35), which, using Eqs. (2.28), (2.29), (3.33), and (3.46), can still be put in the form

$$\hat{A}=\frac{1}{2\pi}\sum_{\mu=0,1}\sum_{m=-\infty}^{+\infty}\sum_{m'=-\infty}^{+\infty}\sum_{m''=-\infty}^{+\infty}\int_{-\pi}^{+\pi}d\theta\frac{\sin\left[\left[m-m'-\frac{\mu}{2}\right]\pi\right]}{\left[m-m'-\frac{\mu}{2}\right]\pi}\times\exp\left[-i2\left[m''+\frac{\mu}{2}\right]\theta\right]A_m(\theta)|m'+m''+\mu\rangle\langle m'-m''|$$
$$=\sum_{\mu=0,1}\sum_{\mu'=0,1}\sum_{m'=-\infty}^{+\infty}\sum_{m''=-\infty}^{+\infty}\int_{-\pi}^{+\pi}d\theta\exp\left[-i2\left[m''+\frac{\mu}{2}\right]\theta\right]a_{m'+\mu'/2}(\theta)|m'+m''+\mu\rangle\langle m'-m''| . \quad (3.51)$$

It is a straightforward exercise to check that the set of Eqs (2.35) and (3.51) is indeed consistent with the set of Eqs. (3.45)–(3.47). These two sets of equations may be regarded as defining a rotational Weyl correspondence that replaces, for $\theta$ and $m$, the Weyl correspondence of Eqs. (2.16) and (2.17), valid for $q$ and $p$. Quite naturally, there is no formal symmetry between $\theta$ and $m$. It is also worth remarking that the expansion of $W_m(\theta,t)$ and $A_m(\theta)$ in terms of $w_{m+\mu/2}(\theta,t)$ and $a_{m+\mu/2}(\theta)$, respectively, as in Eqs. (3.25) and (3.46), provides a most natural way of exhibiting the marked distinction there is between evenness and oddness in the discrete $m$ domain, as can be verified by looking at the kinematic relations that have been established in this section.

## IV. ELEMENTS OF DYNAMICS

### A. Equation of motion for the rotational Wigner function

Following Eq. (3.25), the dynamics of $W_m(\theta,t)$ can be established directly from the dynamics of $w_{m+\mu/2}(\theta,t)$, according to

$$\partial_t W_m(\theta,t)=\tfrac{1}{2}\sum_{\mu=0,1}\sum_{m'=-\infty}^{+\infty}\frac{\sin\left[\left[m-m'-\frac{\mu}{2}\right]\pi\right]}{\left[m-m'-\frac{\mu}{2}\right]\pi}\times\partial_t w_{m'+\mu/2}(\theta,t)\ . \quad (4.1)$$

So, it is the equation of motion for $w_{m+\mu/2}(\theta,t)$ that is going to be derived below. From Eq. (3.26) and the time-dependent Schrödinger equation, written as

$$i\hbar\partial_t\langle m|\psi(t)\rangle=\sum_{m'=-\infty}^{+\infty}\langle m|\hat{H}|m'\rangle\langle m'|\psi(t)\rangle\ , \quad (4.2)$$

it follows that

$$\partial_t w_{m+\mu/2}(\theta,t)=i\frac{1}{\pi\hbar}\sum_{\mu'=0,1}\sum_{m'=-\infty}^{+\infty}\sum_{m''=-\infty}^{+\infty}\exp\left[-i2\left[m'-m''+\frac{\mu}{2}\right]\theta\right]\times[\langle m-m'+m''|\psi(t)\rangle\langle\psi(t)|m+m'+m''+\mu'\rangle\times\langle m+m'+m''+\mu'|\hat{H}|m+m'-m''+\mu\rangle-\langle m-m'+m''|\hat{H}|m+m'+m''+\mu'\rangle\times\langle m+m'+m''+\mu'|\psi(t)\rangle\langle\psi(t)|m+m'-m''+\mu\rangle]\ . \quad (4.3)$$

This last equation can be modified to read

$$\partial_t w_{m+\mu/2}(\theta,t)=i\frac{1}{\pi\hbar}\sum_{\mu'=0,1}\sum_{m'=-\infty}^{+\infty}\sum_{m''=-\infty}^{+\infty}\sum_{n'=-\infty}^{+\infty}\sum_{n''=-\infty}^{+\infty}\left\{\exp\left[-i2\left[m'-m''+\frac{\mu-2\mu\mu'}{2}\right]\theta\right]\delta_{m'-\mu\mu',n''}\delta_{m''+\mu'-\mu\mu',-n'}-\delta_{m'+\mu'-\mu\mu',-n''}\delta_{m''-\mu+\mu\mu',n'}\times\exp\left[i2\left[m'-m''+\frac{\mu-2\mu\mu'}{2}\right]\theta\right]\right\}\times\langle m+m'-n'|\hat{H}|m+m'+n'+\mu+\mu'-2\mu\mu'\rangle\times\langle m+m''-n''|\psi(t)\rangle\langle\psi(t)|m+m''+n''+\mu'\rangle\ , \quad (4.4)$$

which is equivalent to

$$\partial_t w_{m+\mu/2}(\theta,t)=\frac{1}{\pi^2\hbar}\sum_{\mu'=0,1}\sum_{m'=-\infty}^{+\infty}\sum_{m''=-\infty}^{+\infty}\int_{-\pi/2}^{+\pi/2}d\theta'\int_{-\pi/2}^{+\pi/2}d\theta''\sin\left[2\left[m''-\frac{\mu-\mu'}{2}\right]\theta'-2\left[m'+\frac{\mu'-2\mu\mu'}{2}\right]\theta''\right]\times2\sum_{n'=-\infty}^{+\infty}\exp\left[-i2\left[n'+\frac{\mu+\mu'-2\mu\mu'}{2}\right](\theta+\theta')\right]\times\langle m+m'-n'|\hat{H}|m+m'+n'+\mu+\mu'-2\mu\mu'\rangle\times\frac{1}{\pi}\sum_{n''=-\infty}^{+\infty}\exp\left[-i2\left[n''+\frac{\mu'}{2}\right](\theta+\theta'')\right]\times\langle m+m''-n''|\psi(t)\rangle\langle\psi(t)|m+m''+n''+\mu'\rangle\ , \quad (4.5)$$

or to

$$\partial_t w_{m+\mu/2}(\theta,t)=\frac{1}{\pi^2\hbar}\sum_{\mu'=0,1}\sum_{m'=-\infty}^{+\infty}\sum_{m''=-\infty}^{+\infty}\int_{-\pi/2}^{+\pi/2}d\theta'\int_{-\pi/2}^{+\pi/2}d\theta''\sin\left[2\left[m''-\frac{\mu-\mu'}{2}\right]\theta'-2\left[m'+\frac{\mu'-2\mu\mu'}{2}\right]\theta''\right]\times h_{m+m'+(\mu+\mu'-2\mu\mu')/2}(\theta+\theta')w_{m+m''+\mu'/2}(\theta+\theta'',t)\ , \quad (4.6)$$

where Eq. (3.26) has been used and $h_{m+\mu/2}(\theta)$ denotes the function associated with $\hat{H}$ through Eq. (3.47). In order to facilitate the algebra that follows, it is convenient to rewrite Eq. (4.6) as

$$\partial_t w_{m+\mu/2}(\theta,t)=\frac{1}{\pi^2\hbar}\sum_{\mu'=0,1}\sum_{m'=-\infty}^{+\infty}\sum_{m''=-\infty}^{+\infty}\int_{-\pi/2}^{+\pi/2}d\theta'\int_{-\pi/2}^{+\pi/2}d\theta''\,\mathrm{Im}\left\{\exp\left[i2\left[m''-\frac{\mu-\mu'}{2}\right]\theta' -i2\left[m'+\frac{\mu'-2\mu\mu'}{2}\right]\theta''\right]\right\} \times h_{m+m'+(\mu+\mu'-2\mu\mu')/2}(\theta+\theta')w_{m+m''+\mu'/2}(\theta+\theta'',t)\ . \tag{4.7}$$

Now, let the operators $\delta_{+m}$ and $\delta_{-m}$, and their powers $(\delta_{+m})^n$ and $(\delta_{-m})^n$, be defined according to

$$(\delta_{+m})^n=[\ln(1+\Delta_m)]^n=n!\sum_{n'=n}^{\infty}\frac{S_{n'}^{(n)}}{n'!}(\Delta_m)^{n'}\ ,$$
$$(\delta_{-m})^n=[\ln(1-\nabla_m)]^n=n!\sum_{n'=n}^{\infty}\frac{S_{n'}^{(n)}}{n'!}(-\nabla_m)^{n'}\ , \tag{4.8}$$

where $S_{n'}^{(n)}$ denotes the Stirling numbers of the first kind [10] and $\Delta_m$ and $\nabla_m$ are the forward and backward differences, respectively, which applied to a given function $a_{m+\mu/2}(\theta)$ give

$$\Delta_m a_{m+\mu/2}(\theta)=a_{m+1+\mu/2}(\theta)-a_{m+\mu/2}(\theta)\ ,$$
$$\nabla_m a_{m+\mu/2}(\theta)=a_{m+\mu/2}(\theta)-a_{m-1+\mu/2}(\theta)\ . \tag{4.9}$$

Then, for $m'\geq 0$, starting from the Gregory-Newton expansions [11,12]

$$a_{m+m'+\mu/2}(\theta)=\sum_{n'=0}^{\infty}\begin{bmatrix}m'\\ n'\end{bmatrix}(\Delta_m)^{n'}a_{m+\mu/2}(\theta)\ ,$$
$$a_{m-m'+\mu/2}(\theta)=\sum_{n'=0}^{\infty}\begin{bmatrix}m'\\ n'\end{bmatrix}(-\nabla_m)^{n'}a_{m+\mu/2}(\theta) \tag{4.10}$$

and expanding the binomial coefficients using the equality [10]

$$\begin{bmatrix}m'\\ n'\end{bmatrix}=\frac{1}{n'!}\sum_{n=0}^{n'}S_{n'}^{(n)}(m')^n\ , \tag{4.11}$$

it is possible to write [13]

$$a_{m+m'+\mu/2}(\theta)=\exp(m'\delta_{+m})a_{m+\mu/2}(\theta)\ ,$$
$$a_{m-m'+\mu/2}(\theta)=\exp(m'\delta_{-m})a_{m+\mu/2}(\theta)\ . \tag{4.12}$$

These expressions are to be compared with the Taylor expansion

$$a_{m+\mu/2}(\theta+\theta')=\exp(\theta'\partial_\theta)a_{m+\mu/2}(\theta)\ , \tag{4.13}$$

where $\theta'$ may take any real value [14]. In the same way that the introduction, in Sec. III, of variables of the $\mu$ and $\mu'$ type, which are either 0 or 1, has marked a clear cut with the Weyl-Wigner formalism in $q$ and $p$ at the kinematic level, the introduction here of the operators $\delta_{+m}$ and $\delta_{-m}$, reflected below in variables of the $\nu$ and $\nu'$ type, which are either $-1$ or $+1$, is a further step that strongly distinguishes, now at the dynamic level, the Weyl-Wigner formalsim in $\theta$ and $m$.

Applying the results of Eq. (4.12) to the sum

$$\sum_{m'=-\infty}^{+\infty}\exp\left[-i2\left[m'+\frac{\mu'-2\mu\mu'}{2}\right]\theta''\right]h_{m+m'+(\mu+\mu'-2\mu\mu')/2}(\theta+\theta')$$
$$=\exp[-i(\mu'-2\mu\mu')\theta'']\times\left[h_{m+(\mu+\mu'-2\mu\mu')/2}(\theta+\theta')+\sum_{\nu'=-1,+1}\sum_{m'=1}^{\infty}\exp(-i2\nu'm'\theta'')h_{m+\nu'm'+(\mu+\mu'-2\mu\mu')/2}(\theta+\theta')\right]\ , \tag{4.14}$$

which appears in Eq. (4.7), it follows

$$\sum_{m'=-\infty}^{+\infty}\exp\left[-i2\left[m'+\frac{\mu'-2\mu\mu'}{2}\right]\theta''\right]h_{m+m'+(\mu+\mu'-2\mu\mu')/2}(\theta+\theta')$$
$$=\exp[-i(\mu'-2\mu\mu')\theta'']\left[1+\sum_{\nu'=-1,+1}\sum_{m'=1}^{\infty}\exp(m'\delta^h_{\nu'm})\exp(-i2\nu'm'\theta'')\right]h_{m+(\mu+\mu'-2\mu\mu')/2}(\theta+\theta') \tag{4.15}$$

or, still,

$$\sum_{m'=-\infty}^{+\infty}\exp\left[-i2\left[m'+\frac{\mu'-2\mu\mu'}{2}\right]\theta''\right]h_{m+m'+(\mu+\mu'-2\mu\mu')/2}(\theta+\theta')$$
$$=\exp[-i(\mu'-2\mu\mu')\theta'']\left[1+\sum_{\nu'=-1,+1}\sum_{m'=1}^{\infty}\exp\left[i\frac{\nu'}{2}\partial_{\theta''}\delta^h_{\nu'm}\right]\exp(-i2\nu'm'\theta'')\right]h_{m+(\mu+\mu'-2\mu\mu')/2}(\theta+\theta')\ . \tag{4.16}$$

The sum over $m'$ in the right-hand side of Eq. (4.16) can be calculated using the theory of generalized functions [15] and gives

$$\sum_{m'=1}^{\infty}\exp(-i2\nu'm'\theta'')=\sum_{m'=1}^{\infty}\cos(2m'\theta'')-i\nu'\sum_{m'=1}^{\infty}\sin(2m'\theta'')=\tfrac{1}{2}\left[-1+\pi\sum_{n=-\infty}^{+\infty}\delta(\theta''-\pi n)-i\nu'\cot(\theta'')\right], \tag{4.17}$$

so

$$\begin{aligned}\sum_{m'=-\infty}^{+\infty}&\exp\left[-i2\left[m'+\frac{\mu'-2\mu\mu'}{2}\right]\theta''\right]h_{m+m'+(\mu+\mu'-2\mu\mu')/2}(\theta+\theta')\\&=\frac{\pi}{2}\exp[-i(\mu'-2\mu\mu')\theta'']\\&\quad\times\sum_{\nu'=-1,+1}\exp\left[i\frac{\nu'}{2}\partial_{\theta''}\delta^{h}_{\nu'm}\right]\left[\sum_{n=-\infty}^{+\infty}\delta(\theta''-\pi n)-i\frac{\nu'}{\pi}\cot(\theta'')\right]h_{m+(\mu+\mu'-2\mu\mu')/2}(\theta+\theta')\ .\end{aligned} \tag{4.18}$$

In an analogous way,

$$\begin{aligned}\sum_{m''=-\infty}^{+\infty}&\exp\left[-i2\left[m''+\frac{\mu-\mu'}{2}\right]\theta'\right]w_{m+m''+\mu'/2}(\theta+\theta'',t)\\&=\frac{\pi}{2}\exp[-i(\mu-\mu')\theta']\sum_{\nu'=-1,+1}\exp\left[-i\frac{\nu}{2}\partial_{\theta'}\delta^{w}_{\nu m}\right]\left[\sum_{n=-\infty}^{+\infty}\delta(\theta'-\pi n)+i\frac{\nu}{\pi}\cot(\theta')\right]w_{m+\mu'/2}(\theta+\theta'',t)\ .\end{aligned} \tag{4.19}$$

Hence, using Eqs. (4.18) and (4.19), and then integrating by parts in $\theta'$ and $\theta''$, Eq. (4.7) becomes

$$\begin{aligned}\partial_t w_{m+\mu/2}(\theta,t)=\frac{1}{4\hbar}\sum_{\mu'=0,1}\sum_{\nu=-1,+1}\sum_{\nu'=-1,+1}\int_{-\pi/2}^{+\pi/2}d\theta'\int_{-\pi/2}^{+\pi/2}d\theta''\,\mathrm{Im}&\left\{\left[\sum_{n=-\infty}^{+\infty}\delta(\theta'-\pi n)+i\frac{\nu}{\pi}\cot(\theta')\right]\right.\\&\times\left[\sum_{n=-\infty}^{+\infty}\delta(\theta''-\pi n)-i\frac{\nu'}{\pi}\cot(\theta'')\right]\\&\times\exp[i\tfrac{1}{2}(\partial_{\theta'}\delta^{w}_{\nu m}\nu-\nu'\delta^{h}_{\nu'm}\partial_{\theta''})]\\&\left.\times\exp[-i(\mu-\mu')\theta'-i(\mu'-2\mu\mu')\theta'']\right\}\\&\times h_{m+(\mu+\mu'-2\mu\mu')/2}(\theta+\theta')w_{m+\mu'/2}(\theta+\theta'',t)\ .\end{aligned} \tag{4.20}$$

When integrating by parts in $\theta'$ and $\theta''$, it must be borne in mind that the boundary terms appearing at $-\pi/2$ and $+\pi/2$ cancel each other because the integrand in Eq. (4.7) has period $\pi$ both in $\theta'$ and $\theta''$, as can be verified with the help of Eqs. (3.26) and (3.47). Here, the fact that periodicity is naturally taken care of reflects the usefulness of expressing, according to Eqs. (3.25) and (3.46), $W_m(\theta,t)$ and $H_m(\theta)$ in terms of $w_{m+\mu/2}(\theta,t)$ and $h_{m+\mu/2}(\theta)$, respectively, and of working with the latter functions rather than with the former.

Next, considering that

$$\begin{aligned}\exp[i\tfrac{1}{2}(\partial_{\theta'}\delta^{w}_{\nu m}\nu-\nu'\delta^{h}_{\nu'm}\partial_{\theta''})]&\exp[-i(\mu-\mu')\theta'-i(\mu'-2\mu\mu')\theta'']h_{m+(\mu+\mu'-2\mu\mu')/2}(\theta+\theta')w_{m+\mu'/2}(\theta+\theta'',t)\\&=\exp\left[\frac{\mu-\mu'}{2}\nu\delta^{w}_{\nu m}-\frac{\mu'-2\mu\mu'}{2}\nu'\delta^{h}_{\nu'm}\right]\exp[-i(\mu-\mu')\theta'-i(\mu'-2\mu\mu')\theta'']\\&\quad\times\exp[i\tfrac{1}{2}(\partial_{\theta'}\delta^{w}_{\nu m}\nu-\nu'\delta^{h}_{\nu'm}\partial_{\theta''})]h_{m+(\mu+\mu'-2\mu\mu')/2}(\theta+\theta')w_{m+\mu'/2}(\theta+\theta'',t)\ ,\end{aligned} \tag{4.21}$$

and that

$$\begin{aligned}\exp[i\tfrac{1}{2}(\partial_{\theta'}\delta^{w}_{\nu m}\nu-\nu'\delta^{h}_{\nu'm}\partial_{\theta''})]&h_{m+(\mu+\mu'-2\mu\mu')/2}(\theta+\theta')w_{m+\mu'/2}(\theta+\theta'',t)\\&=\exp(i\tfrac{1}{2}L^{h,w}_{\nu,\nu'})\exp(\theta'\partial^{h}_{\theta})\exp(\theta''\partial^{w}_{\theta})h_{m+(\mu+\mu'-2\mu\mu')/2}(\theta)w_{m+\mu'/2}(\theta,t)\ ,\end{aligned} \tag{4.22}$$

where Eq. (4.13) has been used and the operator

$$L^{h,w}_{\nu,\nu'}=\partial^h_\theta\delta^w_{\nu m}\nu-\nu'\delta^h_{\nu' m}\delta^w_\theta \tag{4.23}$$

introduced, Eq. (4.20) can be written as

$$\begin{aligned}\partial_t w_{m+\mu/2}(\theta,t)=\frac{1}{4\hbar}\sum_{\mu'=0,1}\sum_{\nu=-1,+1}\sum_{\nu'=-1,+1}\int_{-\pi/2}^{+\pi/2}d\theta'\int_{-\pi/2}^{+\pi/2}d\theta''\exp\left[\frac{\mu-\mu'}{2}\nu\delta^w_{\nu m}-\frac{\mu'-2\mu\mu'}{2}\nu'\delta^h_{\nu' m}\right]\\ \times\mathrm{Im}\left\{\exp(i\tfrac{1}{2}L^{h,w}_{\nu,\nu'})\left[\sum_{n=-\infty}^{+\infty}\delta(\theta'-\pi n)+i\frac{\nu}{\pi}\cot(\theta')\right]\right.\\ \times\exp[-i(\mu-\mu')\theta']\exp(\theta'\partial^h_\theta)\\ \times\left[\sum_{n=-\infty}^{+\infty}\delta(\theta''-\pi n)-i\frac{\nu'}{\pi}\cot(\theta'')\right]\\ \left.\times\exp[-i(\mu'-2\mu\mu')\theta'']\exp(\theta''\partial^w_\theta)\right\}\\ \times h_{m+(\mu+\mu'-2\mu\mu')/2}(\theta)w_{m+\mu'/2}(\theta,t)\ .\end{aligned} \tag{4.24}$$

At this point, it is useful to define the following operators [16]:

$$\begin{aligned}S_\mu&=\frac{1}{\pi}\int_{-\pi/2}^{+\pi/2}d\theta'\cot(\theta')\sin(\mu\theta')\exp(\theta'\partial_\theta)\ ,\\ C_\mu&=\frac{1}{\pi}\int_{-\pi/2}^{+\pi/2}d\theta'\cot(\theta')\cos(\mu\theta')\exp(\theta'\partial_\theta)\ ,\end{aligned} \tag{4.25}$$

which enable Eq. (4.24) to take the form

$$\begin{aligned}\partial_t w_{m+\mu/2}(\theta,t)=\frac{1}{4\hbar}\sum_{\mu'=0,1}\sum_{\nu=-1,+1}\sum_{\nu'=-1,+1}\exp\left[\frac{\mu-\mu'}{2}\nu\delta^w_{\nu m}-\frac{\mu'-2\mu\mu'}{2}\nu'\delta^h_{\nu' m}\right]\\ \times\mathrm{Im}[\exp(i\tfrac{1}{2}L^{h,w}_{\nu,\nu'})(1+\nu S^h_{\mu-\mu'}+i\nu C^h_{\mu-\mu'})(1-\nu' S^w_{\mu'-2\mu\mu'}-i\nu' C^w_{\mu'-2\mu\mu'})]\\ \times h_{m+(\mu+\mu'-2\mu\mu')/2}(\theta)w_{m+\mu'/2}(\theta,t)\ .\end{aligned} \tag{4.26}$$

This last equation is equivalent to

$$\begin{aligned}\partial_t w_{m+\mu/2}(\theta,t)=\frac{1}{4\hbar}\sum_{\mu'=0,1}\sum_{\nu=-1,+1}\sum_{\nu'=-1,+1}\exp\left[\frac{\mu-\mu'}{2}\nu\delta^w_{\nu m}-\frac{\mu'-2\mu\mu'}{2}\nu'\delta^h_{\nu' m}\right]\\ \times\{\sin(\tfrac{1}{2}L^{h,w}_{\nu,\nu'})[1+\nu S^h_{\mu-\mu'}-\nu' S^w_{\mu'-2\mu\mu'}\\ -\nu\nu'(S^h_{\mu-\mu'}S^w_{\mu'-2\mu\mu'}-C^h_{\mu-\mu'}C^w_{\mu'-2\mu\mu'})]\\ +\cos(\tfrac{1}{2}L^{h,w}_{\nu,\nu'})[\nu C^h_{\mu-\mu'}-\nu' C^w_{\mu-2\mu\mu'}\\ -\nu\nu'(S^h_{\mu-\mu'}C^w_{\mu'-2\mu\mu'}+C^h_{\mu-\mu'}S^w_{\mu'-2\mu\mu'})]\}\\ \times h_{m+(\mu+\mu'-2\mu\mu')/2}(\theta)w_{m+\mu'/2}(\theta,t)\ ,\end{aligned} \tag{4.27}$$

which is a most important result. Indeed, Eq. (4.27) is the equation of motion for $w_{m+\mu/2}(\theta,t)$, and, combined with Eq. (4.1), it describes the dynamics of $W_m(\theta,t)$. Moreover, through Eq. (3.50), it also determines the time evolution of the expectation values of dynamical variables. In principle, for a given Hamiltonian, $h_{m+\mu/2}(\theta)$ can be obtained by Eq. (3.47), and then Eq. (4.27) can be solved for $w_{m+\mu/2}(\theta,t)$. In the same way as it has been pointed out in connection with Eq. (2.21), it is worth noting that the rotational Wigner function representing an energy eigenstate must correspond to a stationary solution of Eq. (4.27), a statement that can be verified using Eq. (3.26).

### B. Particular cases of the equation of motion for the rotational Wigner function

In order to illustrate how to work with Eq. (4.27), this equation is going to be detailed for some important cases. The first type of Hamiltonians to be considered are those that depend only on $\hat{l}$,

$$\hat{H}=f(\hat{l})\ . \tag{4.28}$$

In this case, it is easy to see, with the help of Eqs. (2.27), (2.29), and (3.47), that

$$h_{m+\mu/2}(\theta)=2(1-\mu)f(m\hbar) . \tag{4.29}$$

Then, all terms in Eq. (4.27) involving $\partial_\theta^h$ vanish, and

$$\partial_t w_{m+\mu/2}(\theta,t)=-\frac{1}{2\hbar}\sum_{\mu'=0,1}\sum_{\nu=-1,+1}\sum_{\nu'=-1,+1}\exp\left[\frac{\mu-\mu'}{2}\nu\delta_{\nu m}^w-\frac{\mu'-2\mu\mu'}{2}\nu'\delta_{\nu' m}^f\right]$$
$$\times\left[\sin\left[\frac{\nu'}{2}\delta_{\nu' m}^f\partial_\theta^w\right](1-\nu' S_{\mu'-2\mu\mu'}^w)+\nu'\cos\left[\frac{\nu'}{2}\delta_{\nu' m}^f\partial_\theta^w\right]C_{\mu'-2\mu\mu'}^w\right]$$
$$\times(1-\mu-\mu'+2\mu\mu')f(m\hbar)w_{m+\mu'/2}(\theta,t) . \tag{4.30}$$

The sums over $\mu'$ and $\nu$ become trivial, and therefore

$$\partial_t w_{m+\mu/2}(\theta,t)=-\frac{1}{\hbar}\sum_{\nu'=-1,+1}\exp\left[\frac{\mu}{2}\nu'\delta_{\nu' m}^f\right]\left[\sin\left[\frac{\nu'}{2}\delta_{\nu' m}^f\partial_\theta^w\right](1+\nu' S_\mu^w)+\nu'\cos\left[\frac{\nu'}{2}\delta_{\nu' m}^f\partial_\theta^w\right]C_\mu^w\right]f(m\hbar)w_{m+\mu/2}(\theta,t) . \tag{4.31}$$

Among the Hamiltonians that obey Eq. (4.28) is the free rotator with moment of inertia $I$,

$$\hat{H}=\frac{\hat{l}^2}{2I} , \tag{4.32}$$

in which case

$$f(m\hbar)=\frac{(m\hbar)^2}{2I} . \tag{4.33}$$

From Eqs. (4.8) and (4.9), it is straightforward to see that

$$\nu'\delta_{\nu' m}m^2=2m ,\qquad (\nu'\delta_{\nu' m})^2 m^2=2 , \tag{4.34}$$

and that $(\delta_{+m})^n$ and $(\delta_{-m})^n$ with $n\geq 3$ give zero when applied to the function $m^2$. As a consequence the sum over $\nu'$ in Eq. (4.31) is immediate, and this equation becomes

$$\partial_t w_{m+\mu/2}(\theta,t)=-\frac{\hbar}{2I}\left\{(\delta_{+m}m^2)+\left[\frac{\mu}{2}(\delta_{+m})^2m^2\right]\right\}\times\partial_\theta w_{m+\mu/2}(\theta,t) . \tag{4.35}$$

So, taking into account Eq. (4.34),

$$\partial_t w_{m+\mu/2}(\theta,t)=-\frac{\left[m+\frac{\mu}{2}\right]\hbar}{I}\partial_\theta w_{m+\mu/2}(\theta,t) , \tag{4.36}$$

which is to be compared with Eq. (2.24) for the free particle. Unlike Eq. (2.24), Eq. (4.36) is not equal to its classical counterpart, which is obvious because angular momentum quantization is intrinsic to quantum mechanics and does not have any classical analog.

Another example to be considered is

$$\hat{H}=-\omega\gamma\cos(\hat{\theta}) , \tag{4.37}$$

which may appear in Hamiltonians describing hindered rotators, like the one in Eq. (2.37). Moreover, together with Eq. (4.32), Eq. (4.37) can be used to represent the Hamiltonian of a simple pendulum. The matrix elements $\langle m|\hat{H}|m'\rangle$ corresponding to Eq. (4.37) are given by

$$\langle m|\hat{H}|m'\rangle=-\frac{\omega\gamma}{\pi}\int_{-\pi}^{+\pi}d\theta\exp[-i(m-m')\theta]\cos(\theta)$$
$$=-\frac{\omega\gamma}{2}\delta_{|m-m'|,1} , \tag{4.38}$$

as follows from Eqs. (2.27)–(2.29), and thus Eq. (3.47) yields

$$h_{m+\mu/2}(\theta)=-2\mu\omega\gamma\cos(\theta) . \tag{4.39}$$

Since, in this case, $h_{m+\mu/2}(\theta)$ is independent of $m$, Eq. (4.27) reads, after some algebra,

$$\partial_t w_{m+\mu/2}(\theta,t)=-\frac{\omega\gamma}{\hbar}\sum_{\nu=-1,+1}\exp\left[\frac{1-2\mu}{2}\nu\delta_{\nu m}\right]\left\{\sin\left[\frac{\nu}{2}\delta_{\nu m}\partial_\theta^{\cos}\right][1-(1-2\mu)\nu S_1^{\cos}]+\nu\cos\left[\frac{\nu}{2}\delta_{\nu m}\partial_\theta^{\cos}\right]C_1^{\cos}\right\}$$
$$\times\cos(\theta)w_{m+(1-\mu)/2}(\theta,t) . \tag{4.40}$$

Now, from the definitions in Eq. (4.25),

$$S_1\cos(\theta)=\frac{2}{\pi}\cos(\theta)\int_0^{\pi/2}d\theta'[\cos(\theta')]^2=\tfrac{1}{2}\cos(\theta) ,$$
$$C_1\cos(\theta)=-\frac{2}{\pi}\sin(\theta)\int_0^{\pi/2}d\theta'[\cos(\theta')]^2=-\tfrac{1}{2}\sin(\theta) . \tag{4.41}$$

Using these results in Eq. (4.40),

$$\partial_t w_{m+\mu/2}(\theta,t)=-\frac{\omega\gamma}{2\hbar}\sum_{\nu=-1,+1}\exp\left[\frac{1-2\mu}{2}\nu\delta_{\nu m}\right]\left\{[2-(1-2\mu)\nu]\sin\left[\frac{\nu}{2}\delta_{\nu m}\partial_\theta^{\cos}\right]\cos(\theta)-\nu\cos\left[\frac{\nu}{2}\delta_{\nu m}\partial_\theta^{\sin}\right]\sin(\theta)\right\}$$
$$\times w_{m+(1-\mu)/2}(\theta,t)\ , \tag{4.42}$$

and then performing the explicit calculation of the derivatives with respect to $\theta$, the following equation is derived:

$$\partial_t w_{m+\mu/2}(\theta,t)$$
$$=\frac{\omega\gamma}{2\hbar}\sin(\theta)\{1-2\mu-(2-\mu)\exp[(1-\mu)\delta_{-m}]$$
$$+(1+\mu)\exp(\mu\delta_{+m})\}$$
$$\times w_{m+(1-\mu)/2}(\theta,t)\ . \tag{4.43}$$

This last expression can be further simplified, with the help of Eq. (4.12), to give

$$\partial_t w_{m+\mu/2}(\theta,t)$$
$$=\frac{\omega\gamma}{\hbar}\sin(\theta)[w_{m+(1+\mu)/2}(\theta,t)-w_{m-(1-\mu)/2}(\theta,t)]\ . \tag{4.44}$$

Following the comment regarding Eqs. (4.32) and (4.37) and the simple pendulum, the equation resulting from adding Eqs. (4.36) and (4.44) describes, within the Weyl-Wigner formalism, the rotational motion of the pendulum.

### C. The nonperiodic limit

As expected, the form of Eq. (4.27) is more complex than the form of Eq. (2.21) [17]. In the former, the variables $\mu$, $\mu'$, $\nu$, and $\nu'$ can be said to reflect the two major modifications that have to be introduced in the Weyl-Wigner formalism as a consequence of rotational periodicity, both of which result from the discrete character of the $m$ domain. Such modifications are the need, conveyed by $\mu$ and $\mu'$, to account for evenness and oddness, a point already mentioned in Sec. III, and the need, conveyed by $\nu$ and $\nu'$, to use two difference operators. It is now going to be checked that the formalism developed in this work possesses the correct nonperiodic limit, meaning that all dependence on $\mu$, $\mu'$, $\nu$, and $\nu'$ disappears and, moreover, the results that have been derived for $\theta$ and $m$ reduce to the known results for $q$ and $p$, if the following transformations are made:

$$q=\theta R,\quad p=\frac{m\hbar}{R}\ , \tag{4.45}$$

and

$$|q\rangle=\frac{1}{R^{1/2}}|\theta\rangle\ ,\quad |p\rangle=\left[\frac{R}{\hbar}\right]^{1/2}|m\rangle\ , \tag{4.46}$$

and the limit $R\to\infty$ is then taken [18]. Here $R$ represents the distance to the axis of rotation, so the limit $R\to\infty$ corresponds to the loss of periodicity.

By doing so with Eqs. (3.25) and (3.26), and comparing with Eq. (2.9), it is easy to see that

$$\lim_{R\to\infty} w_{m+\mu/2}(\theta,t)=\lim_{R\to\infty} W_m(\theta,t)=\hbar W(p,q,t)\ . \tag{4.47}$$

It must be noted that the contributions to the nonperiodic limit of the two terms in the second form of Eq. (3.25) are equal, despite the fact that the term containing $w_{m+1/2}(\theta,t)$ does not contribute to the normalization of $W_m(\theta,t)$, as shown in Eq. (3.36). The importance of keeping the contribution of $w_{m+1/2}(\theta,t)$ to $W_m(\theta,t)$, which contribution is associated with oddness, has already been stressed in connection with Eqs. (3.28) and (3.35). Similarly, from Eqs. (3.46) and (3.47),

$$\lim_{R\to\infty} a_{m+\mu/2}(\theta)=\lim_{R\to\infty} A_m(\theta)=A(p,q)\ , \tag{4.48}$$

and it is also straightforward to show that Eq. (3.51) goes over to Eq. (2.16). Next, Eq. (4.23) can be transformed according to

$$\partial_q=\frac{1}{R}\partial_\theta\ ,\quad \partial_p=\frac{R}{\hbar}\nu\delta_{\nu m}\ , \tag{4.49}$$

as follows from Eq. (4.45), and where the second result is established by comparing Eq. (4.12), written now for the continuous variable $p$ taken at every point $m\hbar/R$, with the corresponding Taylor expansion [19]. It can then be checked that, in the limit $R\to\infty$, Eq. (4.27) does become Eq. (2.21). Therefore, in a certain sense, the Weyl-Wigner formalism in $\theta$ and $m$ may be regarded as the general case from which both the Weyl-Wigner formalism in $q$ and $p$ as well as the classical formalism can be derived as limiting cases. It is now particularly clear that the formalism that has been developed for $\theta$ and $m$ cannot be considered as a trivial extension of the Weyl-Wigner formalsim in $q$ and $p$.

## V. ANALYSIS OF A HINDERED ROTATOR

### A. Stationary solution of the equation of motion for the rotational Wigner function and rotational Wigner function for the energy eigenstates

The hindered rotator corresponding to Eq. (2.37) is a nontrivial example for which an analytic treatment can be carried out in order to illustrate the features of the formalism introduced in Secs. III and IV. Moreover, it makes possible a comparison between the known results quoted in Sec. II and the results to be established here. The rotational Wigner function for the energy eigenstates of that rotator $W_{m_0,m}(\theta)$ is going to be derived by solving Eq. (4.27) for its stationary solutions $w_{m_0,m+\mu/2}(\theta)$ and by then introducing the latter in Eq. (3.25). The energy eigenstates are labeled by the parameter $m_0$, shown below to be an integer such that $m_0 \gg 1$, which is consistent with the results given in Sec. II. Recognizing that the first term appearing in the Hamiltonian of Eq. (2.37) is of the type described by Eq. (4.28), and that the second term is equal to the example of Eq. (4.37), and, furthermore, recalling Eq. (2.38), the right-hand side of Eq. (4.31) has to be calculated for

$$f(m\hbar)=|m|\omega\hbar \tag{5.1}$$

and the result has to be added to the right-hand side of Eq. (4.44).

Starting from the definitions in Eq. (4.9) and performing some combinatorial algebra, the following expression, valid for $n \geq 1$, can be established:

$$\begin{aligned}(\Delta_m)^n|m| &= (\nabla_m)^n|m+n| \\ &= \Phi(m)\delta_{n,1} - \Phi(-m-1)\left[\delta_{n,1} + \Phi(m+n-1)2(-1)^{m+n}\begin{bmatrix} n-2 \\ -m-1\end{bmatrix}\right],\end{aligned} \tag{5.2}$$

where $\Phi(x)$ is unity for $x \geq 0$ and is zero otherwise. Hence, from Eqs. (4.8) and (5.2),

$$(\delta_{\nu m})^n|m| = \Phi(\nu m)\delta_{n,1} - \Phi(-\nu m-1)\left[\delta_{n,1} + 2n!\sum_{n'=1-\nu m}^{+\infty}(-1)^{m+n'}\frac{S_{n'}^{(n)}}{n'!}\begin{bmatrix} n'-2 \\ -\nu m-1\end{bmatrix}\right], \tag{5.3}$$

with the sum over $n'$ in Eq. (5.3) stemming from the singular behavior the function $|m|$ exhibits at the origin [20]. Choosing to work at $|m| \gg 1$, such sum is now going to be disregarded, so that

$$(\delta_{\nu m})^n|m| \cong [\Phi(\nu m) - \Phi(-\nu m-1)]\delta_{n,1} . \tag{5.4}$$

It is understood that no fully rigorous mathematical argument has justified this approximation. However, it is to be verified below that the form of $w_{m_0,m+\mu/2}(\theta)$ obtained following such approximation is adequate, as far as the calculation of expectation values of dynamical variables is concerned. In addition, it must be noted that the last equation is valid not only for $|m| \gg 1$, but also for $m=0$, since in this case Eqs. (5.3) and (5.4) are identical. Therefore, using Eqs. (5.1) and (5.4) in Eq. (4.31), and combining the latter with Eq. (4.44), it is possible to write

$$w_{m_0,+1/2}(\theta) = w_{m_0,-1/2}(\theta) \tag{5.5}$$

for $m=0$ and $\mu=0$, and

$$\partial_\theta w_{m_0,m+\mu/2}(\theta) \cong \frac{|m|}{m}\frac{\gamma}{\hbar}\sin(\theta)[w_{m_0,m+(1+\mu)/2}(\theta) - w_{m_0,m-(1-\mu)/2}(\theta)] \tag{5.6}$$

for $|m| \gg 1$. These equations together with Eqs. (3.27) and (3.36), which take here the form

$$w_{m_0,m+\mu/2}(\theta+\pi) = (-1)^\mu w_{m_0,m+\mu/2}(\theta) , \tag{5.7}$$

$$\sum_{m=-\infty}^{+\infty}\int_{-\pi}^{+\pi}d\theta\, w_{m_0,m}(\theta) = 2 , \tag{5.8}$$

define the stationary problem that has to be solved in order to derive $w_{m_0,m+\mu/2}(\theta)$.

So, solutions have to be found for Eq. (5.6), which are real and obey the boundary conditions of Eqs. (5.5) and (5.7) as well as the normalization condition of Eq. (5.8). Changing variables according to

$$\begin{aligned} y &= \frac{2\gamma}{\hbar}\cos(\theta) , \\ k &= 2m+\mu , \\ \Phi(k)Z_k^{(+)}(y) &+ \Phi(-k)Z_k^{(-)}(y) = w_{m_0,m+\mu/2}(\theta) ,\end{aligned} \tag{5.9}$$

where $Z_k^{(+)}(y)$ and $Z_k^{(-)}(y)$ correspond to the two distinct branches $k \gg 1$ and $k \ll -1$, respectively, Eq. (5.6) gives

$$\begin{aligned} 2\partial_y Z_k^{(+)}(y) &\cong Z_{k-1}^{(+)}(y) - Z_{k+1}^{(+)}(y) , \\ 2\partial_y Z_k^{(-)}(y) &\cong Z_{k+1}^{(-)}(y) - Z_{k-1}^{(-)}(y) .\end{aligned} \tag{5.10}$$

The functions $Z_k^{(+)}(y)$ and $Z_k^{(-)}(y)$ are to be linked by the relation

$$Z_{+1}^{(+)}(y) = Z_{-1}^{(-)}(y) , \tag{5.11}$$

and must obey

$$\begin{aligned} Z_k^{(+)}(-y) &= (-1)^k Z_k^{(+)}(y) , \\ Z_k^{(-)}(-y) &= (-1)^k Z_k^{(-)}(y) ,\end{aligned} \tag{5.12}$$

as follows from Eqs. (5.5) and (5.7). The general solutions of Eq. (5.10), which are real and bounded for every $y$ and $k$, can be written as [21]

$$\begin{aligned} Z_k^{(+)}(y) &\cong BJ_{k-\lambda}(y) , \\ Z_k^{(-)}(y) &\cong B'J_{k+\lambda'}(-y) = B'J_{-k-\lambda'}(y) ,\end{aligned} \tag{5.13}$$

where $B$, $B'$, $\lambda$, and $\lambda'$ are constants to be determined, with $\lambda$ and $\lambda'$ integers. Combining Eqs. (5.11) and (5.13), it is easy to see that $B$ and $B'$ must be equal, as well as $\lambda$ and $\lambda'$. Furthermore, Eq. (5.12) implies that $\lambda$ must be even, so it may be replaced by $2m_0$, with $m_0$ an integer. Taking these results into account, and going back to $\theta$ and $m$ with the help of Eq. (5.9), $w_{m_0,m+\mu/2}(\theta)$ can be put in the form

$$w_{m_0,m+\mu/2}(\theta)\cong BJ_{|2m+\mu|-2m_0}\left[\frac{2\gamma}{\hbar}\cos(\theta)\right]. \tag{5.14}$$

Since $|m|\gg 1$, it is seen from Eq. (5.14) that the only values of $m_0$ for which $w_{m_0,m+\mu/2}(\theta)$ is not vanishingly small, and which are thus relevant, are those obeying $m_0\gg 1$. It remains to calculate $B$ making use of Eq. (5.8), which, for $m_0\gg 1$, can be approximated by

$$\frac{1}{B}\cong\int_{-\pi}^{+\pi}d\theta\sum_{m=-\infty}^{+\infty}J_{2m}\left[\frac{2\gamma}{\hbar}\cos(\theta)\right], \tag{5.15}$$

where the sum over $m$ is immediate and gives unity. Consequently,

$$B\cong\frac{1}{2\pi}, \tag{5.16}$$

so that Eq. (5.14) becomes

$$w_{m_0,m+\mu/2}(\theta)\cong\frac{1}{2\pi}J_{|2m+\mu|-2m_0}\left[\frac{2\gamma}{\hbar}\cos(\theta)\right]. \tag{5.17}$$

In order to ascertain that $w_{m_0,m+\mu/2}(\theta)$ in Eq. (5.17) does correspond to an energy eigenstate of the hindered rotator described by the Hamiltonian in Eq. (2.37), the expectation value of the latter in the state represented by $w_{m_0,m+\mu/2}(\theta)$, denoted by $\langle H\rangle_{m_0}$, can be calculated using Eq. (3.50). Thus, putting together Eqs. (3.50), (4.29), (4.39), (5.1), and (5.17), $\langle H\rangle_{m_0}$ may be written as

$$\langle H\rangle_{m_0}\cong\frac{\omega}{4\pi}\sum_{\mu=0,1}\sum_{m=-\infty}^{+\infty}\int_{-\pi}^{+\pi}d\theta[(1-\mu)|m|\hbar-\mu\gamma\cos(\theta)]J_{|2m+\mu|-2m_0}\left[\frac{2\gamma}{\hbar}\cos(\theta)\right]. \tag{5.18}$$

For $m_0\gg 1$, elementary manipulatons transform Eq. (5.18) into

$$\langle H\rangle_{m_0}\cong\frac{\omega\hbar}{\pi}\int_0^{\pi}d\theta\left\{m_0\sum_{m=-\infty}^{+\infty}J_{2m}\left[\frac{2\gamma}{\hbar}\cos(\theta)\right]+\sum_{m=-\infty}^{+\infty}mJ_{2m}\left[\frac{2\gamma}{\hbar}\cos(\theta)\right]\right.$$
$$\left.+\frac{\gamma}{\hbar}\cos(\theta)\sum_{m=-\infty}^{+\infty}J_{2m+1}\left[\frac{2\gamma}{\hbar}\cos(\theta)\right]\right\}. \tag{5.19}$$

In this last equation, the first sum over $m$ gives unity, whereas the other two give zero. Hence

$$\langle H\rangle_{m_0}\cong m_0\omega\hbar, \tag{5.20}$$

confirming that $w_{m_0,m+\mu/2}(\theta)$ corresponds to the energy eigenstate whose energy is given by Eq. (2.39). It is easy to check that this state verifies the uncertainty relation of Eq. (2.26), since the expectation value of $\exp(i\hat{\theta})$ obtained with Eq. (5.17) vanishes, as can be inferred from the foregoing calculation.

Next, using Eq. (5.17) in Eq. (3.25), it follows that

$$W_{m_0,m}(\theta)\cong\frac{1}{4\pi}J_{2(|m|-m_0)}\left[\frac{2\gamma}{\hbar}\cos(\theta)\right]+\frac{1}{(2\pi)^2}\sum_{m'=-\infty}^{+\infty}\frac{(-1)^{m-m'-1}}{(m-m'-\frac{1}{2})}J_{|2m'+1|-2m_0}\left[\frac{2\gamma}{\hbar}\cos(\theta)\right], \tag{5.21}$$

which, for $m_0\gg 1$ and with the help of the equality in Eq. (3.23), takes the form

$$W_{m_0,m}(\theta)\cong\frac{1}{4\pi}J_{2(|m|-m_0)}\left[\frac{2\gamma}{\hbar}\cos(\theta)\right]$$
$$+\frac{1}{\pi^2}\int_0^{\pi/2}d\phi\{\sin[2(m-m_0)\phi]-\sin[2(m+m_0)\phi]\}\sum_{m'=0}^{\infty}\sin[(2m'+1)\phi]J_{2m'+1}\left[\frac{2\gamma}{\hbar}\cos(\theta)\right], \tag{5.22}$$

which, in turn, is equivalent to

$$W_{m_0,m}(\theta)\cong\frac{1}{4\pi}J_{2(|m|-m_0)}\left[\frac{2\gamma}{\hbar}\cos(\theta)\right]+\frac{1}{2\pi^2}\int_0^{\pi/2}d\phi\{\sin[2(m-m_0)\phi]-\sin[2(m+m_0)\phi]\}\sin\left[\frac{2\gamma}{\hbar}\cos(\theta)\sin(\phi)\right]$$
$$=\frac{1}{4\pi}J_{2(|m|-m_0)}\left[\frac{2\gamma}{\hbar}\cos(\theta)\right]-\frac{1}{\pi^2}\int_0^{\pi/2}d\phi\sin(2m_0\phi)\cos(2m\phi)\sin\left[\frac{2\gamma}{\hbar}\cos(\theta)\sin(\phi)\right]. \tag{5.23}$$

For $m \gg 1$ and $m_0 \gg 1$, $\sin[2(m+m_0)\phi]$ becomes a rapidly oscillating function of $\phi$ whose average value is zero, so its contribution to the integral in the first of the forms of Eq. (5.23) may be neglected, and this equation reduces to an expression that does not coincide exactly with the result of Eq. (2.40), but is a factor 2 smaller. This discrepancy is only apparent, being easily explained by the fact that $W_{m_0,m}(\theta)$ in Eq. (2.40) must be considered to be normalized only on the positive half of the $m$ domain, since it has been derived using a Wentzel-Kramers-Brillouin eigenfunction that is valid only for the branch $m \gg 1$. Actually, Eq. (2.40) can be established following a procedure analogous to the one utilized to arrive at Eq. (5.23), but working with that branch alone.

The distributions for $m$ and $\theta$ corresponding to $w_{m_0,m+\mu/2}(\theta)$ in Eq. (5.17) are

$$|\langle m|\psi_{m_0}\rangle|^2 \cong \frac{1}{4\pi}\int_{-\pi}^{+\pi} d\theta\, J_{2(|m|-m_0)}\left[\frac{2\gamma}{\hbar}\cos(\theta)\right] = \frac{1}{2}\left[J_{|m|-m_0}\left[\frac{\gamma}{\hbar}\right]\right]^2 \tag{5.24}$$

and

$$|\langle \theta|\psi_{m_0}\rangle|^2 \cong \frac{1}{4\pi}\sum_{m=-\infty}^{+\infty} J_{2(|m|-m_0)}\left[\frac{2\gamma}{\hbar}\cos(\theta)\right] \cong \frac{1}{2\pi}, \tag{5.25}$$

respectively, as follows from Eqs. (3.34) and (3.35), and where the numerical value of Eq. (5.25) follows for $m_0 \gg 1$. The fact that $w_{m_0,m+\mu/2}(\theta)$ does not contribute to $|\langle m|\psi_{m_0}\rangle|^2$ is a consequence of the general property stated in Eq. (3.34), whereas the fact that it does not contribute to $|\langle \theta|\psi_{m_0}\rangle|^2$ stems from a particular property of the form given in Eq. (5.17). These properties explain why the first term alone of Eq. (5.23) can be retained when calculating $|\langle m|\psi_{m_0}\rangle|^2$ and $|\langle \theta|\psi_{m_0}\rangle|^2$ using Eqs. (2.32) and (2.33) in the same way as pointed out in Sec. II for Eq. (2.40). In addition, the result, also mentioned in Sec. II, according to which the second term of this equation is essential to ensure that $w_{m_0,m}(\theta)$ possesses the correct classical limit, a result that obviously applies also to Eq. (5.23), may be interpreted in the light of the general results derived at the end of Sec. IV and concerning the nonperiodic limit. Indeed, as shown in that section, such term containing $w_{m_0,m+\mu/2}(\theta)$ must be kept if the appropriate nonperiodic limit is to be recovered, which, in turn, guarantees the correct classical limit.

The usefulness of the necessary condition written in Eq. (3.37) can now be illustrated by checking if $w_{m_0,m+\mu/2}(\theta)$ in Eq. (5.17) can indeed represent a pure state, which is here the energy eigenstate of Eq. (2.39). Considering that, always with $m_0 \gg 1$,

$$\frac{1}{4}\sum_{\mu=0,1}\sum_{m=-\infty}^{+\infty}\int_{-\pi}^{+\pi} d\theta [w_{m_0,m+\mu/2}(\theta)]^2 \cong \frac{1}{8\pi^2}\int_{-\pi}^{+\pi} d\theta \sum_{m=-\infty}^{+\infty}\left\{J_m\left[\frac{2\gamma}{\hbar}\cos(\theta)\right]\right\}^2 = \frac{1}{4\pi}, \tag{5.26}$$

it is actually seen that Eq. (3.37) does not hold. Therefore, the results given in Eqs. (5.17) and (5.23) are not fully correct, and more complete forms have to be found for $w_{m_0,m+\mu/2}(\theta)$ and $W_{m_0,m}(\theta)$.

### B. Solution of the time-independent Schrödinger equation and rotational Wigner function for the energy eigenstates

An alternative way to derive $W_{m_0,m}(\theta)$ is to solve the appropriate time-independent Schrödinger equation,

$$\varepsilon\omega\hbar\langle m|\psi_{m_0}\rangle = \sum_{m'=-\infty}^{+\infty}\langle m|\hat{H}|m'\rangle\langle m'|\psi_{m_0}\rangle, \tag{5.27}$$

corresponding to the Hamiltonian of Eq. (2.37), and use the wave function thus derived, $\langle m|\psi_{m_0}\rangle$, to construct $W_{m_0,m}(\theta)$ from Eqs. (3.24), or (3.25) and (3.26). Here $\varepsilon$ is an eigenvalue to be identified below, for the case where $|m| \gg 1$, with the parameter $m_0$ labeling the energy eigenstates according to Eq. (2.39). Proceeding from Eq. (5.27) and taking into account Eqs. (2.37), (2.38), and (4.38), the appropriate time-independent Schrödinger problem follows:

$$\frac{2(|m|-\varepsilon)\hbar}{\gamma}\langle m|\psi_{m_0}\rangle = \langle m-1|\psi_{m_0}\rangle + \langle m+1|\psi_{m_0}\rangle, \tag{5.28}$$

$$-\frac{2\varepsilon\hbar}{\gamma}\langle 0|\psi_{m_0}\rangle = \langle -1|\psi_{m_0}\rangle + \langle +1|\psi_{m_0}\rangle, \tag{5.29}$$

with Eq. (5.29) an eigenvalue equation for $\varepsilon$. This problem is, in itself, a very interesting one [22].

The general solutions of Eqs. (5.28) and (5.29), which are bounded for every $m$, are of the form [21]

$$\langle m|\psi_{m_0}\rangle = DJ_{|m|-\varepsilon}\left[\frac{\gamma}{\hbar}\right], \tag{5.30}$$

where $D$ is a normalization constant and $\varepsilon$ is now a solution of the equation

$$J'_{-\varepsilon}\left[\frac{\gamma}{\hbar}\right] = 0, \tag{5.31}$$

with $J'_\alpha(x)$ denoting the derivative with respect to $x$ of $J_\alpha(x)$. If solutions $\langle m|\psi_{m_0}\rangle$ are to be looked for such that $|m| \gg 1$, then the only values of $\varepsilon$ for which $\langle m|\psi_{m_0}\rangle$ given by Eq. (5.30) does not become vanishingly small are those obeying $\varepsilon \gg 1$. Hence Eq. (5.31) is to be solved for $\varepsilon \gg 1$. A mathematically rigorous asymptotic analysis of the latter equation is possible [23,24], but a simpler approach is adopted here, starting from the relations [21]

$$J_{-\alpha}(x) = \cos(\alpha\pi)J_\alpha(x) - \sin(\alpha\pi)Y_\alpha(x), \tag{5.32}$$

$$J_\alpha(x) \cong \frac{1}{(2\pi\alpha)^{1/2}}\left[\frac{ex}{2\alpha}\right]^\alpha, \quad Y_\alpha(x) \cong -\left[\frac{2}{\pi\alpha}\right]^{1/2}\left[\frac{2\alpha}{ex}\right]^\alpha, \tag{5.33}$$

where $Y_\alpha(x)$ is the Bessel function of the second kind of order $\alpha$ and argument $x$, and the asymptotic approximations in Eq. (5.33) are valid for $\alpha \gg 1$. Thus, combining Eqs. (5.31)–(5.33),

$$\left[\frac{e\gamma}{2\varepsilon\hbar}\right]^{2\varepsilon} \cong 2\tan(\varepsilon\pi) . \tag{5.34}$$

For $\varepsilon \gg 1$, it is readily seen that the solutions of Eq. (5.34) are asymptotic to the positive integers, so $\varepsilon$ can be replaced by $m_0$ and

$$\langle m|\psi_{m_0}\rangle \cong D J_{|m|-m_0}\left[\frac{\gamma}{\hbar}\right] . \tag{5.35}$$

The normalization condition of Eq. (2.30) becomes, considering that $m_0 \gg 1$,

$$\frac{1}{D^2} \cong 2 \sum_{m=-\infty}^{+\infty} \left[J_m\left[\frac{\gamma}{\hbar}\right]\right]^2 , \tag{5.36}$$

whence

$$D \cong \frac{1}{2^{1/2}} . \tag{5.37}$$

So, from Eq. (5.35),

$$\langle m|\psi_{m_0}\rangle \cong \frac{1}{2^{1/2}} J_{|m|-m_0}\left[\frac{\gamma}{\hbar}\right] , \tag{5.38}$$

and, recalling Eqs. (2.28) and (2.29),

$$\begin{aligned}\langle \theta|\psi_{m_0}\rangle &\cong \frac{1}{2\pi^{1/2}} \sum_{m=-\infty}^{+\infty} \exp(im\theta) J_{|m|-m_0}\left[\frac{\gamma}{\hbar}\right] \\ &\cong \frac{1}{\pi^{1/2}}\cos\left[m_0\theta + \frac{\gamma}{\hbar}\sin(\theta)\right] \\ &= \left\{\frac{1}{2\pi} + \frac{1}{2\pi}\cos\left[2m_0\theta + \frac{2\gamma}{\hbar}\sin(\theta)\right]\right\}^{1/2} .\end{aligned} \tag{5.39}$$

Before proceeding, it must be remarked that the distribution $|\langle m|\psi_{m_0}\rangle|^2$ corresponding to Eq. (5.38) is the same as the one in Eq. (5.24), which has been derived from $w_{m_0,m+\mu/2}(\theta)$ in Eq. (5.17). Therefore, the latter gives, for dynamical variables depending on $m$, the same expectation values as $|\langle m|\psi_{m_0}\rangle|^2$ from Eq. (5.38). Moreover, with $m_0 \gg 1$, $|\langle\theta|\psi_{m_0}\rangle|^2$ arising from Eq. (5.39) is the sum of the uniform distribution in Eq. (5.25) with a function of $\theta$ that has a rapidly oscillating component whose average value is zero. Hence, and because Eq. (5.25) stems from Eq. (5.17), it is seen that $w_{m_0,m+\mu/2}(\theta)$ in this equation must yield, for dynamical variables depending on $\theta$ and up to negligible terms, expectation values that are equal to those obtained using $|\langle\theta|\psi_{m_0}\rangle|^2$ from Eq. (5.39), with the possible exception of dynamical variables whose period in $\theta$ is close to that of the rapid oscillations in Eq. (5.39). It is thus verified the adequacy, as far as expectation values are concerned, of the approximation made in going from Eq. (5.3) to Eq. (5.4) when deriving $w_{m_0,m+\mu/2}(\theta)$ from its equation of motion.

Now, making use of Eq. (5.38) in Eq. (3.26), $w_{m_0,m+\mu/2}(\theta)$ reads

$$w_{m_0,m+\mu/2}(\theta) \cong \frac{1}{2\pi} \sum_{m'=-\infty}^{+\infty} \exp\left[-i2\left[m'+\frac{\mu}{2}\right]\theta\right] J_{|m-m'|-m_0}\left[\frac{\gamma}{\hbar}\right] J_{|m+m'+\mu|-m_0}\left[\frac{\gamma}{\hbar}\right] . \tag{5.40}$$

By carefully accounting for the different branches of $|m-m'|$ and $|m+m'+\mu|$ in Eq. (5.40), the latter can be rewritten, for $|m| \gg 1$ and $m_0 \gg 1$, as

$$\begin{aligned} w_{m_0,m+\mu/2}(\theta) \cong{}& \frac{1}{2\pi}\exp\left[i2\left[\left|m+\frac{\mu}{2}\right| - m_0\right]\theta\right] \sum_{m'=-\infty}^{+\infty} \exp(i2m'\theta) J_{|2m+\mu|-2m_0+m'}\left[\frac{\gamma}{\hbar}\right] J_{m'}\left[-\frac{\gamma}{\hbar}\right] \\ &+ \frac{1}{\pi}\cos\left[2\left[\left|m+\frac{\mu}{2}\right| + m_0\right]\theta\right] \sum_{m'=-\infty}^{+\infty} \cos(2m'\theta) J_{|2m+\mu|+m'}\left[\frac{\gamma}{\hbar}\right] J_{m'}\left[\frac{\gamma}{\hbar}\right] \\ &- \frac{1}{\pi}\sin\left[2\left[\left|m+\frac{\mu}{2}\right| + m_0\right]\theta\right] \sum_{m'=-\infty}^{+\infty} \sin(2m'\theta) J_{|2m+\mu|+m'}\left[\frac{\gamma}{\hbar}\right] J_{m'}\left[\frac{\gamma}{\hbar}\right] . \end{aligned} \tag{5.41}$$

The sums over $m'$ appearing in Eq. (5.41) can be performed using the Graf theorem for the addition of Bessel functions [21] and the result is

$$w_{m_0,m+\mu/2}(\theta) \cong \frac{1}{2\pi} J_{|2m+\mu|-2m_0}\left[\frac{2\gamma}{\hbar}\cos(\theta)\right] + \frac{(-1)^m}{\pi}[(1-\mu)\cos(2m_0\theta) - \mu\sin(2m_0\theta)] J_{2m+\mu}\left[\frac{2\gamma}{\hbar}\sin(\theta)\right] . \tag{5.42}$$

The next thing to do is to check if $w_{m_0,m+\mu/2}(\theta)$ given in Eq. (5.42) does verify the necessary condition of Eq. (3.37). After some reduction, the following expression can be established, taking into account that $m_0 \gg 1$:

$$\tfrac{1}{4}\sum_{\mu=0,1}\sum_{m=-\infty}^{+\infty}\int_{-\pi}^{+\pi}d\theta[w_{m_0,m+\mu/2}(\theta)]^2$$
$$\cong\frac{1}{2\pi}+\frac{1}{8\pi^2}\int_{-\pi}^{+\pi}d\theta\cos(4m_0\theta)\sum_{m=-\infty}^{+\infty}\left[\left\{J_{2m}\left[\frac{2\gamma}{\hbar}\sin(\theta)\right]\right\}^2-\left\{J_{2m+1}\left[\frac{2\gamma}{\hbar}\sin(\theta)\right]\right\}^2\right]$$
$$+\frac{1}{2\pi^2}\int_{-\pi}^{+\pi}d\theta\cos(2m_0\theta)\sum_{m=-\infty}^{+\infty}(-1)^m J_{2(m-m_0)}\left[\frac{2\gamma}{\hbar}\cos(\theta)\right]J_{2m}\left[\frac{2\gamma}{\hbar}\sin(\theta)\right]$$
$$-\frac{1}{2\pi^2}\int_{-\pi}^{+\pi}d\theta\sin(2m_0\theta)\sum_{m=-\infty}^{+\infty}(-1)^m J_{2(m-m_0)+1}\left[\frac{2\gamma}{\hbar}\cos(\theta)\right]J_{2m+1}\left[\frac{2\gamma}{\hbar}\sin(\Theta)\right], \quad (5.43)$$

where the equality in Eq. (5.26) has been used. The Graf theorem can be utilized both to provide an adequate expansion for the Bessel functions in the second term of Eq. (5.43) and to perform the sums over $m$ appearing in the last two terms. Carrying out some more algebra it is then possible to write

$$\tfrac{1}{4}\sum_{\mu=0,1}\sum_{m=-\infty}^{+\infty}\int_{-\pi}^{+\pi}d\theta[w_{m_0,m+\mu/2}(\theta)]^2$$
$$\cong\frac{1}{2\pi}+\frac{1}{\pi}J_{2m_0}\left[\frac{2\gamma}{\hbar}\right]+\frac{1}{4\pi}\left[\sum_{m=-\infty}^{+\infty}J_{2m_0-m}\left[\frac{2\gamma}{\hbar}\right]J_m\left[\frac{2\gamma}{\hbar}\right]\right]^2, \quad (5.44)$$

which, making use of the Neumann theorem for the addition of Bessel functions [21], is equivalent to

$$\tfrac{1}{4}\sum_{\mu=0,1}\sum_{m=-\infty}^{+\infty}\int_{-\pi}^{+\pi}d\theta[w_{m_0,m+\mu/2}(\theta)]^2$$
$$\cong\frac{1}{2\pi}+\frac{1}{\pi}J_{2m_0}\left[\frac{2\gamma}{\hbar}\right]+\frac{1}{4\pi}\left[J_{2m_0}\left[\frac{2\gamma}{\hbar}\right]\right]^2. \quad (5.45)$$

Consequently, the form in Eq. (5.42) satisfies Eq. (3.37) up to terms that are vanishingly small for $m_0 \gg 1$. Indeed, according to Eq. (5.33), Eq. (5.45) may be written as

$$\tfrac{1}{4}\sum_{\mu=0,1}\sum_{m=-\infty}^{+\infty}\int_{-\pi}^{+\pi}d\theta[w_{m_0,m+\mu/2}(\theta)]^2 \cong\frac{1}{2\pi}+O(m_0^{-2m_0}). \quad (5.46)$$

It can further be shown, for the form of $w_{m_0,m+\mu/2}(\theta)$ given in Eq. (5.42), that

$$\tfrac{1}{2}\sum_{m=-\infty}^{+\infty}\int_{-\pi}^{+\pi}d\theta\, w_{m_0,m}(\theta)\cong 1+J_{2m_0}\left[\frac{2\gamma}{\hbar}\right]$$
$$\cong 1+O(m_0^{-2m_0}), \quad (5.47)$$

so the normalization condition of Eq. (3.36) holds true up to terms that can be neglected for $m_0 \gg 1$.

Thus, putting together Eqs. (3.25) and (5.42) and using the equality in Eq. (3.23), the following results for $W_{m_0,m}(\theta)$:

$$W_{m_0,m}(\theta)\cong\frac{1}{4\pi}J_{2(|m|-m_0)}\left[\frac{2\gamma}{\hbar}\cos(\theta)\right]+\frac{(-1)^m}{2\pi}\cos(2m_0\theta)J_{2m}\left[\frac{2\gamma}{\hbar}\sin(\theta)\right]$$
$$-\frac{1}{\pi^2}\int_0^{\pi/2}d\phi\sin(2m_0\phi)\cos(2m\phi)\sin\left[\frac{2\gamma}{\hbar}\cos(\theta)\sin(\phi)\right]$$
$$-\frac{1}{\pi^2}\sin(2m_0\theta)\int_0^{\pi/2}d\phi\cos(2m\phi)\sin\left[\frac{2\gamma}{\hbar}\sin(\theta)\cos(\phi)\right]. \quad (5.48)$$

Provided that $|m| \gg 1$ and $m_0 \gg 1$, the preceding equation gives the rotational Wigner function for the energy eigenstates of the hindered rotator described by the Hamiltonian of Eq. (2.37), which eigenstates have the energies given in Eq. (2.39). This result is valid for both branches $m \gg 1$ and $m \ll -1$. Furthermore, and up to terms that are of order $O(m_0^{-2m_0})$, it is normalized according to Eq. (2.34), obeys the necessary condition for a pure state of Eq. (3.37), and yields the appropriate expectation values of dynamical variables if used in Eq. (2.36).

## VI. SUMMARY AND CONCLUSIONS

A comprehensive study has been presented on the Weyl-Wigner formulation of quantum mechanics in the case of rotational motion. The ensemble of elements on the Weyl-Wigner formalism for rotation-angle and angular-momentum variables has been extended, and the implications for the formalism of rotational periodicity and angular-momentum quantization have been investigated. Particular attention has been paid to discreteness, and two of its consequences have been emphasized: the importance of evenness and oddness, and the need to use difference instead of differential operators. These two consequences have been shown to strongly distinguish the Weyl-Wigner formalism for rotation-angle and angular-momentum variables from the well-known Weyl-Wigner formalism for Cartesian-position and linear-momentum variables. Consequently, it has become clear that the first of these formalisms cannot be regarded as a mere extension of the second, thus reflecting the fact that the two types of variables are intrinsically different in quantum mechanics.

The rotational Wigner function has been derived as the only bilinear form of the state vector that is real, has the natural invariances for rotational motion, and yields the correct distributions for the rotation-angle and angular-momentum variables as well as the appropriate expression for the transition probability between states. The conditions for its uniqueness have been thus established. Its properties have been investigated in detail, having been shown that it is uniformly bounded. The rotational Wigner function and the associated correspondence between quantum operators and classical-like functions have been explored and have been written, as well as the kinematic relations they obey, in such a way as to reflect the marked difference existing, in the discrete domain of the angular-momentum eigenvalues, between evenness and oddness. Such difference is an intrinsic feature of discreteness that has been encountered throughout and has been taken advantage of in order to provide a most natural way to account for periodicity. This has proven to be particularly useful in deriving the dynamics of the rotational Wigner function.

The equation of motion for this function has been established using the derivative, which acts on the continuous rotation-angle variable, and the forward and backward differences, which act on the discrete angular-momentum variable. A further intrinsic feature of discreteness has been thus introduced, which lies in the fact that two difference operators are necessary in a discrete domain, whereas one differential operator suffices in a continuous domain. The equation of motion for the rotational Wigner function, which has revealed a more complex structure than the equation of motion for the well-known Wigner function, has been detailed for some important Hamiltonian forms, namely, those that depend on the angular-momentum variable alone, including, in particular, the free rotator, and those that are in the cosine of the rotation-angle variable. Moreover, it has been shown that the Weyl-Wigner formalism for rotation-angle and angular-momentum variables possesses the correct nonperiodic limit and that it properly reduces to the Weyl-Wigner formalism for Cartesian-position and linear-momentum variables.

A detailed analysis has been provided of a hindered rotator whose Hamiltonian consists of two terms: one in the absolute value of the angular-momentum variable and the other in the cosine of the rotation-angle variable. The rotational Wigner function representing the energy eigenstates of this rotator has been analytically derived within the approximation of a very large absolute value of the angular-momentum variable. This has been done following two distinct methods: by obtaining the stationary solutions of the equation of motion for the rotational Wigner function, as well as by solving the time-independent Schrödinger equation and using the wave function thus obtained to construct the rotational Wigner function. Such analysis has been carried out to illustrate the features of the formalism that has been developed.

## ACKNOWLEDGMENT

Support by the Commission of the European Communities under Euratom Grant No. B 89000563 is gratefully acknowledged.

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[1] S. de Groot, *La Transformation de Weyl et la Fonction de Wigner: Une Forme Alternative de la Mécanique Quantique* (Les Presses de l'Université de Montréal, Montréal, 1974).

[2] N. L. Balazs and B. K. Jennings, Phys. Rep. **104**, 347 (1984).

[3] M. Hillery, R. F. O'Connel, M. O. Scully, and E. P. Wigner, Phys. Rep. **106**, 121 (1984).

[4] P. Carruthers and M. M. Nieto, Rev. Mod. Phys. **40**, 411 (1968).

[5] M. V. Berry, Philos. Trans. R. Soc. London Ser. A **287**, 237 (1977).

[6] N. Mukunda, Am. J. Phys. **47**, 182 (1979).

[7] Whenever necessary, a superscript is used on an operator symbol to designate the function to which the operator is applied. For example, $\partial_q^H$ in Eq. (2.21) designates the derivative of $H(p,q)$ with respect to $q$.

[8] Actually, Eq. (2.35) of the present work cannot be found in Ref. [6] but it can be derived from Eq. (4.8) there provided, after rewriting it with the help of Eqs. (3.3), (3.5), (3.8), and (4.6) therein.

[9] It is worth remarking that the apparently evident transformation $r=2m-m'-m''$ and $s=m'-m''$ cannot be used instead of Eq. (3.15), due to the impossibility of inverting it to express $m'$ and $m''$ in terms of $r$ and $s$ when $r+s$ is odd. In other words, in this transformation $r$ and $s$ are not independent variables, since $r+s$ must be even.

[10] K. Goldberg, M. Newman, and E. Haynsworth, in *Handbook of Mathematical Functions,* edited by M. Abramowitz and I. A. Stegun (Dover, New York, 1965), p. 821.

[11] C. Lanczos, *Linear Differential Operators* (Van Nostrand, London, 1961).

[12] It must be noted that the series of Eq. (4.10) are necessarily convergent, since all terms with $n'>m'$ vanish, as a consequence of the fact that $\binom{m'}{n'}=0$ for $n'>m'$. It is also important to remark that difference operators are used here to set up series expansions of functions of discrete

variables and not, as it is their common use and detailed in Ref. [11], to treat problems of equidistant interpolation of functions of continuous variables.

[13] For all relevant functions $a_{m+\mu/2}(\theta)$, it is assumed that $(\delta_{+m})^n a_{m+\mu/2}(\theta)$ and $(\delta_{-m})^n a_{m+\mu/2}(\theta)$ exist for all orders $n$, much in the same way as the existence of $(\partial_\theta)^n a_{m+\mu/2}(\theta)$ is assumed for all orders $n$. Actually, the series resulting from applying the operators defined in Eq. (4.8) to $a_{m+\mu/2}(\theta)$ are not necessarily convergent, since a resummation process is involved in going from Eq. (4.10) to Eq. (4.12), and the equivalence between these two equations presupposes the convergence of all series concerned.

[14] For the purpose of comparing the series expansions given in Eqs. (4.12) and (4.13), these equations can be put in the suggestive forms $a_{m\pm m'+\mu/2}(\theta)=\exp(m'\delta_{\pm m})a_{m+\mu/2}(\theta)$ and $a_{m+\mu/2}(\theta\pm\theta')=\exp(\pm\theta'\partial_\theta)a_{m+\mu/2}(\theta)$, with $m'\geq 0$ and $\theta'\geq 0$. It is thus seen that the two operators $\delta_{+m}$ and $\delta_{-m}$ are necessary in the discrete $m$ domain, whereas the operator $\partial_\theta$ is sufficient in the continuous $\theta$ domain. In this work, $\delta_{+m}$ and $\delta_{-m}$ have been defined with the help of the forward and backward differences $\Delta_m$ and $\nabla_m$. Alternatively, they can be defined using the two fundamental operators of central differencing, which are discussed in Ref. [11] and are equal to $\Delta_m-\nabla_m$ and $\frac{1}{2}(\Delta_m+\nabla_m)$.

[15] I. M. Gel'fand and G. E. Shilov, *Generalized Functions* (Academic, San Diego, 1964), Vol. 1.

[16] It is worth pointing out that integrals involving $\cot(\theta')$, a function which has a nonintegrable singularity at the origin, are to be calculated after being canonically regularized as discussed in Ref. [15].

[17] It is interesting to note that nontrivial modifications in the Weyl-Wigner formalism for $q$ and $p$ are also introduced when the spin variables are taken into account, as in Ref. [1].

[18] This limit must not be confused with the classical limit $\hbar\rightarrow 0$.

[19] The second result of Eq. (4.49) is known in numerical analysis and can be found in Ref. [10] in connection with the Stirling numbers of the first kind. Once more, the convergence of all series involved is assumed.

[20] It is interesting to note that the singular behavior of $|m|$ at the origin is felt at every $m$, whereas the singular behavior of $|x|$, with $x$ a continuous variable, remains localized at the origin.

[21] F. W. J. Olver, in *Handbook of Mathematical Functions* (Ref. [10]), p. 355.

[22] Similar problems can be found in Ref. [4], in connection with the obtention of the minimum-uncertainty states for the uncertainty relations involving the number and the sine or cosine operators.

[23] M. J. Coulomb, Bull. Sci. Math. (in French) **60**, 297 (1936).

[24] Actually, in Ref. [23] it is shown that the zeros of $J_\alpha(x)$, considered as a function of $\alpha$, are asymptotic to the negative integers. Following a similar demonstration, the same result can be shown for $J'_\alpha(x)$.