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Rigid rotor in phase space

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Angular momentum is an important concept in physics, and its phase space properties are important in various applications. In this work a phase space analysis of angular momentum is made starting from its classical definition, and its quantum properties are obtained by imposing the uncertainty principle. The kinetic energy operator is derived, but its part have a different interpretation from that in the standard treatment. The rigid rotor is discussed and its phase space representation is shown. The true rigid rotor is defined and its phase space properties are also discussed.

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I. INTRODUCTION

Angular momentum is a very important concept in the dynamics of particles and within quantum mechanics its properties are very well understood [1] . One example where the theory has direct application is the rigid rotor model, which is the basis for understanding rotational spectroscopy and collisions of molecules. These processes are described by quantum dynamics, but there are circumstances when classical dynamics is used as an alternative. For example, rotational cross sections for two colliding molecules in principle can be calculated from quantum mechanics, but often it is a challenging task. Classical mechanics, on the other hand, is relatively simple to use, but there are several problems in its implementation, say, to calculate atom-molecule collision cross sections. The basic problem is how the initial conditions are selected and the final results analyzed. For example, if one says that a molecule is in the rotational state with quantum numbers $l=3$ and $m=2$ then the question is what to choose for the initial orientation and angular velocity to adequately represent it. An analogous problem has been analyzed for collisions involving only vibrational energy exchange in atom-molecule collisions, where it was shown how to select initial conditions that adequately represent a particular vibrational state of the molecule. A recipe was suggested from which transition probabilities were successfully calculated [2] from classical mechanics; by that it is meant that initial conditions were selected from a prescribed phase space density but the dynamics is calculated from the classical equations of motion.

The problem is therefore how to choose a set of initial positions and velocities for a particle so that on average its angular momentum has given l and m values. In other words, what is needed is a function $f_{l,m}(\vec{r},\vec{p})$ with the property that the following averages are obtained:

$$\langle(\vec{r}\times\vec{p})^2\rangle=\int d^3r d^3p (\vec{r}\times\vec{p})^2 f_{l,m}(\vec{r},\vec{p})=\hbar^2 l(l+1),$$

$$\langle\vec{r}\times\vec{p}\rangle=\int d^3r d^3p \;\; \vec{r}\times\vec{p} \;\; f_{l,m}(\vec{r},\vec{p})=\hbar m \;\; \hat{z}. \tag{1}$$

In classical mechanics the function $f_{l,m}(\vec{r},\vec{p})$ is interpreted as a statistical weight from which the position and momentum are selected. It should be noted that it is not necessary that $f_{l,m}(\vec{r},\vec{p})$ is a positive function, as long as these averages are obtained. In practice this means that initial conditions are randomly selected from $|f_{l,m}(\vec{r},\vec{p})|$ and if N sets are chosen then the averages are approximately

$$\langle(\vec{r}\times\vec{p})^2\rangle\approx\frac{\sum_{j=1}^{N}(\vec{r}_j\times\vec{p}_j)^2\,\mathrm{sgn}[f_{l,m}(\vec{r}_j,\vec{p}_j)]}{\sum_{j=1}^{N}\mathrm{sgn}[f_{l,m}(\vec{r}_j,\vec{p}_j)]},$$

and similarly for the angular momentum. The function $\mathrm{sgn}[f_{l,m}(\vec{r}_j,\vec{p}_j)]$ is the sign of $f_{l,m}(\vec{r}_j,\vec{p}_j)$ for the set of initial conditions $(\vec{r}_j,\vec{p}_j)$. However, a much more stringent condition is that the function $f_{l,m}(\vec{r},\vec{p})$ is stationary. The meaning of this can be demonstrated by a simple example. If a particle of mass M is free and the set of its initial conditions is $(\vec{r}_j,\vec{p}_j)$ then its position after time t is $\vec{r}=\vec{r}_j+(\vec{p}_j/M)t$ and its velocity $\vec{v}=\vec{p}_j/M$. From these values one can calculate a new distribution function $g(\vec{r},\vec{p})$, by requiring it to have the properties previously described for the function $f_{l,m}(\vec{r},\vec{p})$. Stationarity requires that the two functions are identical for any time t. This restriction is very important, for obvious reasons, and it is sufficient to dismiss a large number of *ad hoc* distributions.

The most obvious starting point would be the wave function for a particle in a particular angular momentum state, which in the coordinate space is $\psi_{l,m}(\vec{r})=\chi_{n,l}(r)Y_{l,m}(\theta,\phi)$, where $Y_{l,m}(\theta,\phi)$ is the spherical harmonic. Likewise, in momentum space the wave function is $\varphi_{l,m}(\vec{p})=\omega_{n,l}(p)Y_{l,m}(\theta_p,\phi_p)$, where θ_p and ϕ_p are angles of the momentum. One could then form the function $f_{l,m}(\vec{r},\vec{p})=|\chi_{n,l}(r)Y_{l,m}(\theta,\phi)|^2|\omega_{n,l}(p)Y_{l,m}(\theta_p,\phi_p)|^2$ from which the initial position vector and momentum could be selected, except that neither are the averages (1) obtained nor is the condition of stationarity for the function $f_{l,m}(\vec{r},\vec{p})$ satisfied, which is easily proved. Therefore this simple idea fails, and this is because one basic difference between classical and quantum dynamics was not taken into account: classical dynamics is defined in the phase space, while quantum dynamics is in either the coordinate or momentum space. The simple product that was suggested for the distribution $f_{l,m}(\vec{r},\vec{p})$ only reflects this: it says that the initial conditions in the phase space are determined as the product of the distributions from the coordinate and momentum space, which are independent. What is needed is a formulation of quantum mechanics in phase space, and then one would possibly be able to satisfy the two conditions above. The earliest attempt in this direction was by Wigner [3], who looked for a function $\rho(\vec{r},\vec{p},t)$ with the property

$$P(\vec{r},t)=|\psi(\vec{r},t)|^2=\int d^3p\ \rho(\vec{r},\vec{p},t),$$

$$Q(\vec{p},t)=|\varphi(\vec{p},t)|^2=\int d^3r\ \rho(\vec{r},\vec{p},t) \tag{2}$$

and obtained what is known as the Wigner function

$$\rho(\vec{r},\vec{p},t)=\frac{1}{\pi^3\hbar^3}\int d^3q\, e^{2i\vec{p}\cdot\vec{q}/\hbar}\psi^*(\vec{r}+\vec{q},t)\psi(\vec{r}-\vec{q},t), \tag{3}$$

which is regarded as an extension of quantum mechanics into the phase space. This definition inevitably results in nonuniqueness of the extension [4], because there is a large class of phase space functions that are defined by the requirements (2). Another attempt to formulate quantum mechanics in phase space is due to Moyal [5,6], whose main objective was to give it a sound statistical foundation. The starting point is postulate observables as operators, and to postulate that for each set of commuting observables there is a set of noncommuting observables. Together they form a complete set of observables. For these observable (operators) one forms a function from which the characteristic function of statistical theory for a given quantum state ψ is obtained as a matrix element. By the Fourier transform, Moyal obtained a distribution that becomes to the Wigner function if the observables are coordinates and momenta. Common to both approaches is that the principles of quantum mechanics are assumed, although the Moyal analysis is more general. Can the Wigner function be used for the distribution $f_{l,m}(\vec{r},\vec{p})$? It is not clear that the averages (1) are obtained; in fact, as will be shown later, they are only partly obtained. Furthermore, it is also not clear that the stationarity condition is satisfied; however, the Wigner function is stationary under the quantum time evolution for the stationary wave function, which is $\psi(\vec{r},t)=\psi_0(\vec{r})e^{-iEt/\hbar}$. The Wigner function has been used in various applications and its properties investigated [7–21], but its true significance is when the connection with classical dynamics is sought. This is achieved by the standard assumption that classical dynamics is the limit of quantum dynamics when $\hbar\rightarrow 0$. It can be shown in general (a one-dimensional problem is discussed for the moment) that the Wigner function satisfies the equation [19,20]

$$\frac{\partial\rho}{\partial t}+\frac{p}{m}\frac{\partial\rho}{\partial x}+\frac{\partial V}{\partial x}\frac{\partial\rho}{\partial p}=-\frac{1}{2i}\int_{-\infty}^{\infty}dy\, e^{ipy}G(x,y)\psi^*\times(x-\hbar y/2,t)\psi(x+\hbar y/2,t)$$

where

$$G(x,y)=\sum_{n=1}^{\infty}\frac{V^{(2n+1)}(x)}{2^{2n}(2n+1)!}(\hbar y)^{2n+1},$$

and in this limit the inhomogeneous term vanishes. It also vanishes if the potential is quadratic, irrespective of this limit. The homogeneous equation is the Liouville equation, which determines the time evolution of the phase space density $\rho(\vec{r},\vec{p},t)$, and it is solved using the classical equations of motion.

Despite this apparently very important connection between quantum and classical dynamics, there are at least two remarks that one can make about this approach. It is desirable for understanding the quantum-classical connection to learn more about the foundations of quantum principles, because we are quite familiar with the classical. Strictly speaking, that goal was not achieved because with either the Wigner or Moyal formulation of the phase space nothing can be learned about quantum principles, because they are the starting point anyway. The second remark concerns the limit of the phase space density when $\hbar\rightarrow 0$, which should also be taken, not only the limit for the inhomogeneous term. For stationary states it can be shown that [13]

$$\rho(\vec{r},\vec{p})\underset{\hbar\rightarrow 0}{=}\delta(H-E_0)=\delta\left[\frac{p^2}{2m}+V(r)-E_0\right]$$

where E_0 is a fixed energy. This form greatly restricts the possible phase space densities from among those stationary solutions that are obtained from the Liouville equation. However, it is consistent with the accepted view, which is based on the correspondence principle: the quantum goes over to the classical solution for large quantum numbers (the proof of this is straightforward but not elaborated here).

The classical-quantum connection can be examined starting from entirely classical principles [22,23], and this, as will be shown, allows much greater flexibility in the application of classical dynamics to quantum problems. One starts from the Liouville equation in classical dynamics, and the argument on which one bases its use is quite straightforward: initial conditions for a particle are never accurately determined, in which case its precise trajectory has no meaning, only the probabilities for its position in the course of time. For example, to claim that the position of the Earth is accurately determined is nonsense, and therefore prediction of its position accurately in the next, say, million years is not possible, especially if perturbation from other planets is taken into account. However, it is possible to predict the probability of finding it at a certain position after (almost) any length of time. Therefore one starts by formulating classical mechanics as a statistical theory (it should be strongly emphasized that *statistical* does not imply *many* particles but the probability for a single particle), in contrast to the attempt by Moyal, whose principal aim was to formulate quantum mechanics as a statistical theory. In other words, one particle in the phase space is not a point but an extended density, which takes into account all uncertainties in determining its whereabouts. For a particle of mass m this equation is

$$\partial_t\rho(\vec{r},\vec{p},t)+\frac{\vec{p}}{m}\cdot\vec{\nabla}_r\rho(\vec{r},\vec{p},t)+\vec{F}\cdot\vec{\nabla}_p\rho(\vec{r},\vec{p},t)=0 \tag{4}$$

where $\vec{F}$ is the force on the particle and $\vec{p}$ is its momentum. The index of the operator $\vec{\nabla}$ designates the variable with respect to which the derivatives are taken. For the particular case when the phase space density is stationary, which means that $\partial_t\rho(\vec{r},\vec{p},t)=0$, the solution is a function of the form $\rho(\vec{r},\vec{p},t)=f(h_1,h_2,h_3,\ldots)$, where f is an arbitrary function and h_i are dynamic invariants of the classical equations of motion. One of them is the Hamiltonian for the particle, and others are components of the angular momentum if the force $\vec{F}$ is centrally symmetric. There are other invariants but they will be mentioned later. These phase space densities, like any other solution of the Liouville equation, lack a very important ingredient in order to be regarded also as quantum solutions. This ingredient is the restriction on the possible phase space densities, and it is in the form of the uncertainty principle

$$\Delta x \quad \Delta p_x \geqslant \hbar/2$$

for any Cartesian coordinate. The standard deviations Δx and Δp are calculated from the phase space density. Mathematically speaking, selecting phase space densities according to this restriction is a very well defined problem and it is solved within a Fourier analysis. They are obtained in the form of the convolution [25]

$$\rho(\vec{r},\vec{p},t)=\frac{1}{\pi^3\hbar^3}\int d^3q\, e^{2i\vec{p}\cdot\vec{q}/\hbar}\, f^*(\vec{r}+\vec{q},\,t)f(\vec{r}-\vec{q},t) \tag{5}$$

which is also recognized as the Wigner function. The function f is arbitrary, but if the phase space density satisfies the Liouville equation then it satisfies the equation [24]

$$i\hbar \quad \partial_t f=-\frac{\hbar^2}{2m}\Delta f+Vf \tag{6}$$

where $\vec{F}=-\vec{\nabla}V$, and the potential is not required to be harmonic (for a general potential parametrization of the phase space density is more elaborate).

The common point between the Wigner and Moyal approaches and the one that starts from classical principles is the function (3) or (5); however, it is an almost arbitrary function in the former case (because there is no reason to choose it from many other functions) but a convolution in the latter. Apart from that common point there are fundamental differences between the two approaches; the former starts from quantum principles and the latter from classical. One manifestation of that is the attitude toward the uncertainty relationship, which in the quantum case it is not considered a principle because it is derived from other ones, while in the classical case it is assumed to be a fundamental principle from which the basic dynamics equation of quantum mechanics (6) is derived. One could cite other fundamental differences between the two approaches, but one is that of simplicity. In the Wigner-Moyal approach one needs all the postulates used in the formulation of quantum mechanics, about whose number there is no general consensus, but in the approach from classical mechanics one needs only the three Newton postulates and the uncertainty postulate. One could question the meaning of the uncertainty principle, but one could equally question the meaning of the observable-operator or wave-particle dualism postulates in the formulation of quantum mechanics. Other advantages that one gains by starting from classical principles and not from the quantum phase space formulation of Wigner and Moyal will be explicitly manifested in the following sections. In particular, it is not clear how to derive the phase space density for the true rigid rotor, which is done in this work, other than by starting from classical principles.

There is one conceptual problem in the attempt to merge classical dynamics with the uncertainty principle. Without the latter, solutions of the Liouville equation are phase space probability densities, and as such they always have positive values. As soon as one imposes a restriction in the form of the uncertainty principle this feature is lost and one often ends with a phase space density that has positive and negative values. This is the price to be paid for imposing that restriction, and its physics is justified on the grounds that the uncertainty principle makes it impossible to measure the phase space probability density precisely. One talks then about the phase space density, whose properties are exactly the same as for the probability density. However, all measurable quantities, e.g., probability density for the coordinates only, must have physically acceptable values.

In Eq. (6) one recognizes the Schrödinger equation, the basic equation of quantum mechanics. Therefore the steps in classical mechanics described produce identical results as in quantum mechanics, provided the initial condition for the phase space density is calculated from the parametrization (5). Using these principles, first the angular momentum for a three-dimensional harmonic oscillator will be analyzed.

II. HARMONIC OSCILLATOR IN THREE DIMENSIONS

Stationary phase space densities for a three-dimensional harmonic oscillator are analyzed assuming that the average

$$\vec{L}=\int d^3r\, d^3p \;\; \vec{r}\times\vec{p}\rho(\vec{r},\vec{p}) \tag{7}$$

has a given value. The starting point is the phase space density which is parametrized as (5), where the functions ψ are chosen in the form $\psi=r^lY_{l,\mu}(\theta,\phi)R_{n,l}(r)$ $=Y_{l,\mu}(x,y,z)R_{n,l}(r)$, where θ and ϕ are spherical angles and r is the radial coordinate. The indices n, l, and μ are

TABLE I. Phase space density for the ground vibrational state of a harmonic oscillator for the first few values of angular momentum numbers. The appropriate angular momentum and its modulus squared are given. Definition of the variables is given in the text.

$l,\ \mu$	$\rho_{0,l,\mu}\pi^3 e^E$	$\langle\vec{L}\rangle$	$\langle L^2\rangle$
0,0	1	0	$0+3/2$
1,0	$-1+2E_z$	0	$1\times2+3/2$
1,1	$-1+E-E_z+2L_z$	$1\ \hat{z}$	$1\times2+3/2$
2,0	$1-(2/3)(E+3E_z)+(1/3)(E-3E_z)^2+(8/3)L^2-4L_z^2$	0	$2\times3+3/2$
2,1	$(1-2E_z)(1-E+E_z-2L_z)$	$1\ \hat{z}$	$2\times3+3/2$
2,2	$-1+(1/2)[E-E_z-2(1-L_z)]^2$	$2\ \hat{z}$	$2\times3+3/2$

integers (in further analysis units are used in which $m=\hbar=1$ and the frequency of the oscillator is $\omega=1$), $Y_{l,\mu}(\theta,\phi)$ is the spherical harmonic, and

$$R_{n,l}(r)=N_1F_1\left(-n,l+\frac{3}{2};r^2\right)e^{-r^2/2}$$

where N is a normalization constant and ${}_1F_1(a,b;z)$ is the hypergeometric function. The phase space density is now

$$\begin{aligned}\rho_{n,l,\mu}(\vec{r},\vec{p})=\frac{1}{\pi^3}\int d^3q\, e^{2i\vec{p}\cdot\vec{q}}\, &Y^*_{l,\mu}(x+q_x,y+q_y,z+q_z)\\ &\times R_{n,l}(|\vec{r}+\vec{q}|)Y_{l,\mu}(x-q_x,y-q_y,z-q_z)\\ &\times R_{n,l}(|\vec{r}-\vec{q}|,)\end{aligned}\tag{8}$$

which in general does not have a simple explicit form, but it has a few nice features. It is stationary, which means that its form does not change with respect to classical time evolution. In other words, if the classical solution for the trajectory is

$$\vec{r}=\vec{r}_0\cos(t)+\vec{p}_0\sin(t)$$

then

$$\begin{aligned}\rho(\vec{r},\vec{p},t)&=\rho_{n,l,\mu}[\vec{r}\cos(t)-\vec{p}\sin(t),\vec{r}\sin(t)+\vec{p}\cos(t)]\\ &=\rho_{n,l,\mu}(\vec{r},\vec{p}).\end{aligned}$$

This means that the phase space density is a function of the dynamic invariants of the harmonic oscillator. One set of these are elements of the energy tensor ($\frac{1}{2}$ is omitted for simplicity) $E_{i,j}=p_ip_j+x_ix_j$, $i,j=1,2,3$ (the indices designate the Cartesian components x, y, and z), and the other set are the components of the angular momentum $x_i\ p_j-x_j\ p_i$, $i\neq j$. Of course, any other combination of these basic invariants is possible, e.g., the total angular momentum squared. Which ones are present in the phase space density (8) is determined by explicit calculation, and the first few for the ground vibrational ($n=0$) state are given in Table I. The symbols represent the following quantities: $E=p^2+r^2$, $E_z=p_z^2+z^2$, $L^2=(yp_z-zp_y)^2+(zp_x-xp_z)^2+(xp_y-yp_x)^2$, and $L_z=xp_y-yp_x$. These are dynamic invariants for the harmonic oscillator, and therefore the phase space density is indeed stationary.

From the phase space densities one can calculate the total angular momentum (7) and its squared modulus from

$$L^2=\int d^3r\, d^3p(\vec{r}\times\vec{p})^2\rho(\vec{r},\vec{p}).$$

Their values are given in Table I and as expected the angular momentum is the same as from quantum analysis: it has only the z component and its value is μ. However, the angular momentum squared is not equal to $l(l+1)$, as expected from the quantum treatment, but differs by 3/2. The same is true for other than $n=0$ states, as shown in Table II. In fact, the most surprising finding is that the states with $l=0$, which are normally associated with zero angular momentum, have the value 3/2 for the angular momentum squared. The question is where this discrepancy comes from. The simplest answer is that the classical analysis is not correct, because it surely must violate certain rules that are not consistent with the quantum mechanical ones. However, this answer is not correct, because if one writes the momentum squared as p^2

TABLE II. Phase space density for the first excited vibrational state of a harmonic oscillator for the first few values of angular momentum numbers. The appropriate angular momentum and its modulus squared are given. Definition of the variables is given in the text.

$l,\ \mu$	$\rho_{0,l,\mu}\pi^3 e^E$	$\langle\vec{L}\rangle$	$\langle L^2\rangle$
0,0	$1-(1/3)(4E-2E^2+8L^2)$	0	$0+3/2$
1,0	$-1+(2/5)(2E-E^2+9E_z-8EE_z+2E^2E_z+12L^2-8E_zL^2-8L_z^2)$	0	$1\times2+3/2$
1,1	$-1+(1/5)(13E-10E^2+2E^3-9E_z+8EE_z-2E^2E_z+16L^2-8EL^2$ $+8E_zL^2+10L_z-8EL_z+4E^2L_z-16L^2L_z+8L_z^2)$	$1\ \hat{z}$	$1\times2+3/2$

$=p_r^2+p_\theta^2+p_\phi^2$, where the components of the momentum are given with respect to the vector $\vec{r}$, then its average for the function $\psi=\Theta(\theta,\phi)R(r)$ is

$$\langle p^2\rangle=\frac{1}{\pi^3}\int d^3r\,dp_r\,dp_\theta\,dp_\phi(p_r^2+p_\theta^2+p_\phi^2)\times\int dq_r\,dq_\theta\,dq_\phi\,e^{2i(p_rq_r+p_\theta q_\theta+p_\phi q_\phi)}\times\Theta^*(\theta_+,\phi_+)R(r_+)\Theta(\theta_-,\phi_-)R(r_-),$$

where

$$r_\pm=\sqrt{(r\pm q_r)^2+q_\theta^2+q_\phi^2},$$

$$\cos\theta_\pm=\frac{\hat{z}\cdot(\vec{r}\pm\vec{q})}{|\vec{r}\pm\vec{q}\,|}=\frac{(r\pm q_r)\cos\theta\pm q_\theta\sin\theta}{\sqrt{(r\pm q_r)^2+q_\theta^2+q_\phi^2}}, \qquad (9)$$

$$e^{i\phi_\pm}=\frac{(\vec{r}\pm\vec{q})\cdot(\hat{x}+i\hat{y})}{|\vec{r}\pm\vec{q}\,|\sin\theta_\pm}=\frac{(r\pm q_r)\sin\theta\mp q_\theta\cos\theta\pm iq_\phi}{|\vec{r}\pm\vec{q}\,|\sin\theta_\pm}e^{i\phi}.$$

After a straightforward but lengthy calculation of the integrals, one obtains

$$\langle p^2\rangle=-\int d^3r\,\psi^*(\vec{r})\frac{1}{r^2}\left[\frac{d}{dr}\left(r^2\frac{d}{dr}\right)+\frac{1}{\sin(\theta)}\frac{\partial}{\partial\theta}\left(\sin(\theta)\frac{\partial}{\partial\theta}\right)+\frac{1}{\sin^2(\theta)}\frac{\partial^2}{\partial\phi^2}\right]\psi(\vec{r}),$$

which is the correct answer for the kinetic energy operator (up to a prefactor, which was not taken into account). In the standard interpretation the angular part is then associated with the angular momentum squared operator, which indeed gives zero for angular momentum squared for the $l=0$ states. Therefore the procedure of deriving the kinetic energy operator is correct, but then the question is where the analysis that produced the results in Tables I and II is inconsistent with the quantum interpretation. To answer this question one explicitly calculates the average of $p_\Omega^2=p_\theta^2+p_\phi^2$, which is the classical angular part of the momentum squared. For simplicity its average will be calculated for the $l=0$ state.

By definition,

$$\langle p_\Omega^2\rangle=\frac{1}{4\pi^4}\int d^3r\,dp_r\,dp_\theta\,dp_\phi(p_\theta^2+p_\phi^2)\times\int dq_r\,dq_\theta\,dq_\phi\,e^{2i(p_rq_r+p_\theta q_\theta+p_\phi q_\phi)}\times R[\sqrt{(r+q_r)^2+q_\theta^2+q_\phi^2}]R[\sqrt{(r-q_r)^2+q_\theta^2+q_\phi^2}],$$

where the integration over p_r and q_r is calculated first, then p_θ^2 and p_ϕ^2 are replaced by derivatives in the variables q_θ and q_ϕ that act on the exponential function, respectively, and after partial integration over the same variables one obtains

$$\langle p_\Omega^2\rangle=-\frac{1}{16\pi^3}\int d^3r\,dp_\theta\,dp_\phi\int dq_\theta\,dq_\phi\,e^{2i(p_\theta q_\theta+p_\phi q_\phi)}\times(\partial_{q_\theta}^2+\partial_{q_\phi}^2)[R^2(\sqrt{r^2+q_\theta^2+q_\phi^2})].$$

After integration over the variables p_θ and p_ϕ the only nonzero contribution is

$$\langle p_\Omega^2\rangle=-\frac{1}{4\pi}\int d^3r\,R(r)\frac{1}{r}\partial_rR(r).$$

In fact, the average of the angular momentum squared (which is $L^2=r^2p_\Omega^2$) is

$$\langle L^2\rangle=-\int_0^\infty dr\,r^3R(r)\partial_rR(r)=\frac{3}{2},$$

which is precisely the value in Tables I and II. Furthermore, the result is independent of the radial function, which indicates that this is a universal number. In order to check the correctness of the result one calculates the average of the radial part of the momentum squared, and the result is

$$\langle p_r^2\rangle=-\frac{1}{4\pi}\int d^3r\,R(r)\left[\partial_r^2R(r)+\frac{1}{r}\partial_rR(r)\right].$$

Together with the angular part one obtains the radial part of the kinetic energy operator

$$T_r=-\frac{1}{r^2}\partial_r(r^2\partial_r).$$

which is the correct answer. Therefore, there is no discrepancy between the quantum expression for the kinetic energy and the classical treatment in this work; the difference is in the interpretation of its parts. According to the results in this work one should interpret the radial kinetic energy operator as

$$T_r=-\partial_r^2-\frac{1}{r}\partial_r$$

while

$$T_\Omega=-\frac{1}{r}\partial_r-\frac{1}{r^2}\left[\frac{1}{\sin(\theta)}\frac{\partial}{\partial\theta}\left(\sin(\theta)\frac{\partial}{\partial\theta}\right)+\frac{1}{\sin^2(\theta)}\frac{\partial^2}{\partial\phi^2}\right]$$

is the operator for the angular momentum squared.

Further confirmation of this comes from calculating the average angular momentum explicitly. For $l=0$ states it is given by

$$\langle\vec{L}\rangle=\langle L_z\rangle\hat{z}=\frac{\hat{z}}{4\pi^4}\int d^3r\,dp_r\,dp_\theta\,dp_\phi\,rp_\phi\sin(\theta)\times\int dq_r\,dq_\theta\,dq_\phi\,e^{2i(p_rq_r+p_\theta q_\theta+p_\phi q_\phi)}R(r_+)R(r_-),$$

which is easily shown to be zero. This is no contradiction with the previous finding, because the zero of the angular momentum is the result of cancellations of the contributions from the two signs of p_ϕ, rather than the modulus of the angular momentum being zero. One can therefore calculate the angular momentum by averaging over only one sign of p_ϕ, because the average over the other gives the same result but with the opposite sign, and the sum total is zero. This average is

$$\langle L_z^+\rangle = \frac{1}{4\pi^4}\int d^3r\, dp_r\, dp_\theta \sin(\theta)\int_0^\infty dp_\phi\, r p_\phi \times \int dq_r\, dq_\theta\, dq_\phi\, e^{2i(p_r q_r + p_\theta q_\theta + p_\phi q_\phi)} \times R(r_+)R(r_-)$$

and after evaluating most of the integrals one gets

$$\langle L_z^+\rangle = -\frac{1}{8i\pi^2}\int d^3r\, r\sin(\theta)\int_0^\infty dp_\phi\int dq_\phi\, e^{2ip_\phi q_\phi}\partial_{q_\phi} \times R^2(\sqrt{r^2+q_\phi^2}).$$

By using the relationship

$$\int_0^\infty dp_\phi\, e^{2ip_\phi q_\phi} = \pi\delta(2q_\phi) + i\mathrm{P}\left(\frac{1}{2q_\phi}\right),$$

where P designates the principal value of the integral, we obtain

$$\langle L_z^+\rangle = -\frac{i}{8i\pi^2}\int d^3r\, r\sin(\theta)\ \ \mathrm{P}\left[\int dq_\phi\, R(\sqrt{r^2+q_\phi^2}) \times R'(\sqrt{r^2+q_\phi^2})\frac{1}{\sqrt{r^2+q_\phi^2}}\right].$$

The principal value can be omitted because the integrand is not singular, in which case

$$\langle L_z^+\rangle = \frac{1}{4}\int dr\, r^2R^2(r) = \frac{1}{4}.$$

The value of the z component of the angular momentum, which gets contributions from the space $p_\phi > 0$, is independent of the radial function $R(r)$, the same result as before.

III. RIGID ROTOR

The rigid rotor in classical physics is a very well defined object, but one could argue that it is also in quantum physics. Unfortunately, as will be shown, the two definitions do not have the same meaning. Intuition, which is essentially classical, defines a rigid object as one that does not have breathing (radial) motion. Objects that appear to qualify as rigid are diatomic molecules (at least many of them), which is supported by the approximations in their quantum description. The Schrödinger equation for the nuclear motion in a diatomic molecule is

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\psi}{\partial r}\right) + \frac{1}{r^2\sin(\theta)}\frac{\partial}{\partial\theta}\left(\sin(\theta)\frac{\partial\psi}{\partial\theta}\right) + \frac{1}{r^2\sin^2(\theta)}\frac{\partial^2\psi}{\partial\phi^2}\right] + V(r)\quad\psi,$$

where m is the reduced mass of the diatomic molecule and $V(r)$ is the internuclear potential. Typically, this potential has a deep minimum displaced from the origin by the distance r_0 (the bond length), which for modeling purposes is approximated by $(m/2)\omega^2(r-r_0)^2$. The ground state wave function in this potential has the width a, and its relationship to the bond length is $r_0 \gg a$. Under these circumstances the radial coordinate in the angular part of the kinetic energy operator is approximated by the fixed value r_0, in which case the wave function factors as $\psi = 1/rR(r)\Theta(\theta,\phi,t)e^{-iE_0t/\hbar}$, where E_0 is the ground state energy of the molecule. The angular function then satisfies the equation

$$i\hbar\frac{\partial\Theta(\theta,\phi,t)}{\partial t} = T_{rot}\Theta(\theta,\phi,t) + W(\theta,\phi,t)\Theta(\theta,\phi,t) \tag{10}$$

where

$$T_{rot} = -\frac{\hbar^2}{2mr_0^2}\left[\frac{1}{\sin(\theta)}\frac{\partial}{\partial\theta}\left(\sin(\theta)\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2(\theta)}\frac{\partial^2}{\partial\phi^2}\right]$$

and $W(\theta,\phi,t)$ represents interactions of the molecule that depend on the angles only (say, a dipole in the electric field).

The unique feature of Eq. (10) is that it depends only on the angle variables, the orientation angles of the molecule, and in this sense it is called the equation for the rigid rotor. The operator T_{rot} then represents the kinetic energy operator for the rigid rotor, which has the discrete spectrum

$$T_{rot}Y_{l,m}(\theta,\phi) = \frac{\hbar^2}{2mr_0^2}l(l+1)Y_{l,m}(\theta,\phi),$$

$$l = 0,1,2,\ldots,\qquad m = -l,-l+1,\ldots,l,$$

where $Y_{l,m}(\theta,\phi)$ are spherical harmonics, the eigenfunctions of the rigid rotor. However, this is far from being true, if one has the image of the classical rigid rotor in mind. Although in the previous derivation the dynamics in the angle variables is decoupled from the dynamics in the radial variable this is not sufficient to call the molecule a rigid rotor. It is also necessary to prove that the radial component of the momentum for the relative motion of the two atoms is decoupled from its angular ones, and to show this one needs to calculate the momentum space wave function. This function for a stationary rotational state of the "rigid rotor" is

$$\varphi(\vec{p}) = \int d^3r\, \frac{1}{r} R(r) Y_{l,m}(\theta,\phi) e^{i\vec{p}\cdot\vec{r}}$$
$$= (2\pi)^{3/2} i^l Y_{l,m}(\theta_p,\phi_p) \frac{1}{\sqrt{p}} \int_0^\infty dr\, r^{1/2} R(r) J_{l+1/2}(pr) \tag{11}$$

where the expansion of the plane wave in spherical coordinates was used. Decoupling of the radial component p_r from the angular ones p_θ and p_ϕ is therefore not possible because $p = \sqrt{p_r^2 + p_\theta^2 + p_\phi^2}$, while the spherical angles θ_p and ϕ_p are related to the same components in a complicated way. Therefore it cannot be assumed that the theoretical model that was just described represents a rigid rotor.

Analysis in phase space is more revealing, but it is somewhat approximate. It was mentioned that around $r = r_0$ the potential is very well approximated by a harmonic, in which case the entire wave function for the diatomic molecule is

$$\phi_l(\vec{r}) = Ne-(r-r_0)^2/2a^2 Y_{l,m}(\theta,\phi)$$

where the $1/r$ coefficient was assumed to be constant. The phase space density is then

$$\rho_{l,m}(\vec{r},\vec{p}) = \frac{N^2}{\pi^3} \int d^3q\, e^{2i\vec{p}\cdot\vec{q}} Y^*_{l,m}(\theta_+,\phi_+)$$
$$\times Y_{l,m}(\theta_-,\phi_-) e^{-(|\vec{r}+\vec{q}|-r_0)^2/2a^2 - (|\vec{r}-\vec{q}|-r_0)^2/2a^2}$$

where the angles $\theta_\pm$ and $\phi_\pm$ are defined in Eq. (9). The rigid rotor model assumption implies that $q \ll r$, and if spherical coordinates are used for the vector $\vec{q} = q_r\hat{r} + q_\theta\hat{\theta} + q_\phi\hat{\phi}$ then the exponent of the harmonic oscillator function is approximately

$$\frac{(|\vec{r}+\vec{q}|-r_0)^2}{2a^2} + \frac{(|\vec{r}-\vec{q}|-r_0)^2}{2a^2} \sim \frac{(r-r_0)^2}{a^2}$$
$$+ \frac{q_r^2}{a^2}\left(1 - \frac{q_\theta^2+q_\phi^2}{r_0^2}\right) + \frac{(q_\theta^2+q_\phi^2)^2}{4a^2r_0^2} + O(q^6),$$

where, in the expansion coefficients, except in the leading one, we set $r = r_0$. By recalling that this expansion is in the exponent, it follows that the range of $|q_r|$ within which it significantly contributes to the phase space density is of order a; however, the range of $\sqrt{q_\theta^2+q_\phi^2}$ is of order $\sqrt{ar_0}$. This means that $|q_r| \ll \sqrt{q_\theta^2+q_\phi^2}$, in which case the phase space density is approximately

$$\rho_{l,m}(\vec{r},\vec{p}) = \frac{2r_0a^2N^2}{\pi^{5/2}} e^{-(r-r_0)^2/a^2 - p_r^2a^2} \int_{-\infty}^{\infty} dq_\theta \int_{-\infty}^{\infty} dq_\phi$$
$$\times e^{2i\sqrt{2ar_0}(p_\theta q_\theta + p_\phi q_\phi) - (q_\theta^2+q_\phi^2)^2}$$
$$\times \Theta_{l,m}(r_0,\theta,\phi,0,\sqrt{2ar_0}q_\theta,\sqrt{2ar_0}q_\phi)$$

where the angular function $\Theta_{l,m}$ is shorthand for the product of two functions $Y_{l,m}(\theta_\pm,\phi_\pm)$. Dependence of the angular function on the radial variable q_r is also neglected, in which case the phase space density parametrizes as the product of the function for the radial variables and the function for the angular. The angular phase space density is now defined as

$$\rho^\Omega_{l,m}(\theta,\phi,p_\theta,p_\phi) = \frac{2ar_0}{\pi^2} \int dq_\theta\, dq_\phi$$
$$\times e^{2i\sqrt{2ar_0}(p_\theta q_\theta + p_\phi q_\phi) - (q_\theta^2+q_\phi^2)^2}$$
$$\times \Theta_{l,m}(r_0,\theta,\phi,0,\sqrt{2ar_0}q_\theta,\sqrt{2ar_0}q_\phi) \tag{12}$$

and appears to describe the rigid rotor because it is independent of the radial variables. However, this conclusion is false because the phase space density depends on the radial parameter a, and in this respect it depends on the radial dynamics. Because of this feature the rigid rotor will be called "soft."

The average of the angular momentum squared now has the value

$$\langle L^2 \rangle = \int \rho^\Omega_{l,m}(\theta,\phi,p_\theta,p_\phi) r_0^2 (p_\theta^2 + p_\phi^2) = l(l+1)$$

where the constant term 3/2 that was obtained in the previous section is missing. This is expected because coupling with the radial motion was neglected. Another property of the angular phase space density is

$$\int_{-\infty}^{\infty} dp_\theta \int_{-\infty}^{\infty} dp_\phi\, \rho^\Omega_{l,m}(\theta,\phi,p_\theta,p_\phi)$$
$$= \Theta_{l,m}(r_0,\theta,\phi,0,0,0) = |Y_{l,m}(\theta,\phi)|^2 \tag{13}$$

which shows that it correctly describes the essentials of the angular momentum. Its explicit form for $l = m = 0$ is given by

$$\rho^\Omega_{0,0}(\theta,\phi,p_\theta,p_\phi) = \frac{ar_0}{\pi^2} \int_0^\infty dq\, q J_0(2\sqrt{2ar_0}pq) e^{-q^4},$$

which does not have an explicit analytic expression. However, its shape is simple, as shown in Fig. 1. For the rotational state $l = 1$ and $m = 0$ the angular phase space density is

$$\rho^\Omega_{1,0}(\theta,\phi,p_\theta,p_\phi)$$
$$= \frac{6ar_0}{4\pi^3} \int_{-\infty}^{\infty} dq_\theta \int_{-\infty}^{\infty} dq_\phi e^{2i\sqrt{2ar_0}(p_\theta q_\theta + p_\phi q_\phi) - (q_\theta^2+q_\phi^2)^2}$$
$$\times \frac{\cos^2\theta - 2\epsilon q_\theta^2 \sin^2\theta}{1 + 2\epsilon q_\theta^2 + 2\epsilon q_\phi^2} \sim \left(\cos^2\theta + \frac{1}{4r_0^2}\partial^2_{p_\theta} + \frac{\cos^2\theta}{4r_0^2}\partial^2_{p_\phi}\right)$$
$$\times \int_0^\infty dq\, q J_0(2\sqrt{2ar_0}pq) e^{-q^4}$$

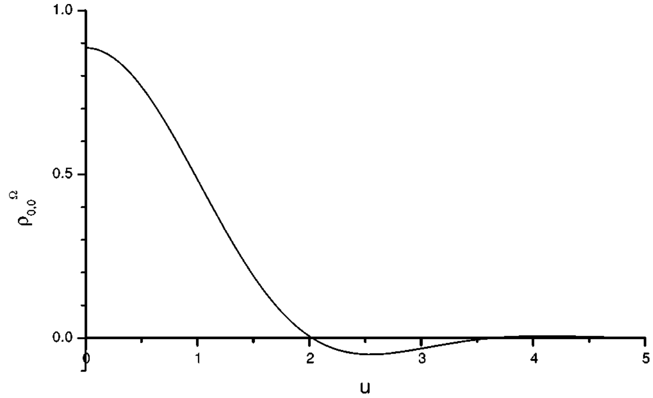

FIG. 1. Phase space density for "soft" rigid rotor, for angular momentum indices $l=m=0$.

where $\epsilon = a/r_0$, and in the last step only the terms up to order ϵ were retained. Similarly the phase space density for $l=1$ and $m=1$ is

$$\rho^{\Omega}_{1,1}(\theta,\phi,p_\theta,p_\phi) \sim \left(\sin^2\theta + \frac{\sin\theta}{r_0}\partial_{p_\phi} + \frac{1}{4r_0^2}\partial^2_{p_\theta} + \frac{1}{4r_0^2}\partial^2_{p_\phi} + \frac{\sin^2\theta}{4r_0^2}\partial^2_{p_\phi}\right)\int_0^\infty dq\, qJ_0 \times (2\sqrt{2ar_0}pq)e^{-q^4}.$$

These phase space densities, except $\rho^{\Omega}_{0,0}$, are time dependent, which means that they are not functions of only the dynamic invariants of the rigid rotor, e.g., $p^2 = p_\theta^2 + p_\phi^2$ and $p_\phi \sin\theta$. Thus, for example, the terms in $\rho^{\Omega}_{1,0}(\theta,\phi,p_\theta,p_\phi)$ that cannot be represented by invariants are

$$\rho^{\Omega}_{1,0}(\theta,\phi,p_\theta,p_\phi) = \cos^2\theta \int_0^\infty dq\, qJ_0(2\sqrt{2ar_0}pq)e^{-q^4} - \frac{\cos^2\theta}{pr_0^2}\sqrt{\frac{ar_0}{2}}\int_0^\infty dq\, q^2 J_1 \times (2\sqrt{2ar_0}pq)e^{-q^4}.$$

The explicit time dependence of the phase space density is obtained from the time dependence of the angle θ,

$$\cos\theta = \cos\theta_0 \cos\frac{tp_0}{mr_0} - \frac{p_\theta^0}{p_0}\sin\theta_0 \sin\frac{tp_0}{mr_0},$$

where θ_0, p_θ^0, and p_0 are the initial values of these variables. In the phase space density $\cos\theta$ is replaced by

$$\cos\theta_t = \cos\theta\cos\frac{tp}{mr_0} + \frac{p_\theta}{p}\sin\theta\sin\frac{tp}{mr_0}$$

and the time dependence of the probability density (13) is calculated from

$$\int_{-\infty}^{\infty} dp_\theta \int_{-\infty}^{\infty} dp_\phi\, \rho^{\Omega}_{1,0}(\theta,\phi,p_\theta,p_\phi)$$

$$\sim \int_{-\infty}^{\infty} dp_\theta \int_{-\infty}^{\infty} dp_\phi \cos^2\theta \int_0^\infty dq\, qJ_0(2\sqrt{2ar_0}pq)e^{-q^4}$$

$$= \frac{\pi}{32ar_0}(1+\cos^2\theta) - \frac{\pi m r_0}{8\sqrt{2ar_0}}(3\cos^2\theta - 1)\partial_t \times \int_0^{t/mr_0\sqrt{2ar_0}} dq\, \frac{qe^{-q^4}}{\sqrt{t^2/2am^2r_0^3 - q^2}}.$$

The first part is time independent, while the second goes to zero after the time interval $t > mr_0\sqrt{2ar_0}$, which is typically of the order $10^{-13}-10^{-14}$ sec for diatomic molecules. Therefore the probability density starts as Eq. (13) but its limiting value is constant, although not in the form of the squared modulus of the spherical harmonic.

IV. TRUE RIGID ROTOR

The previous discussion revealed great difficulty in formulating the concept of a rigid rotor in quantum theory. This was manifested as an inability to formulate a phase space density that involves only the parameters for the rotational degrees of freedom. It does not help to take the limit $a \to 0$ in Eq. (12) because that would imply infinite dispersion of the variables p_θ and p_ϕ, which only reflects the fact that the radial and angular components of the momentum are interrelated. There is, however, a way of formulating the true rigid rotor, but it should be done by following the formulation of quantum mechanics suggested in the Introduction. One starts from the Liouville equation in spherical coordinates, which for a free particle is

$$\partial_t\rho - \frac{p_\theta}{mr}\partial_\theta\rho + \frac{p_\phi}{mr\sin\theta}\partial_\phi\rho + \frac{p_r}{m}\partial_r\rho - \frac{1}{mr} \times \left(\frac{p_\phi^2\cos\theta}{\sin\theta} + p_r p_\theta\right)\partial_{p_\theta}\rho - \frac{p_\phi}{mr}\left(-p_\theta\frac{\cos\theta}{\sin\theta} + p_r\right)\partial_{p_\phi}\rho + \left(\frac{p_\theta^2}{mr} + \frac{p_\phi^2}{mr}\right)\partial_{p_r}\rho = 0,$$

and the rigid rotor assumption implies that the phase space density is r and p_r independent. This means that the Liouville equation for the rigid rotor is

$$\partial_t\rho - \frac{p_\theta}{mr}\partial_\theta\rho + \frac{p_\phi}{mr\sin\theta}\partial_\phi\rho + \frac{p_\phi}{mr}\frac{\cos\theta}{\sin\theta}(p_\theta\partial_{p_\phi}\rho - p_\phi\partial_{p_\theta}\rho) = 0 \qquad (14)$$

where r is constant. It can easily be verified that if the phase space density is a function of the form $\rho(\theta,\phi,p_\theta,p_\phi,t) = F(p_\theta^2 + p_\phi^2, p_\phi\sin\theta)$, where F is an arbitrary function, then it is time independent. An additional requirement is that the phase space density should be in accordance with the uncertainty principle, which is achieved by straightforward generalization of the rule that was used before. The phase space density is therefore parametrized as

$$\rho(\theta,\phi,p_\theta,p_\phi,t)=\frac{1}{\pi^2}\int d^2q\, e^{2i(p_\theta q_\theta+p_\phi q_\phi)}\Theta^* \times(\theta_+,\phi_+)\ \Theta(\theta_-,\phi_-), \tag{15}$$

where the angular functions will be determined for a particular case when the solutions of the Liouville equation (14) are stationary, i.e., $\partial_t\rho=0$. The relevant variables were defined in Eq. (9). The parametrization (15) is replaced in the Liouville equation (14), and by using transformations of the kind

$$p_\theta\rho(\theta,\phi,p_\theta,p_\phi)=-\frac{1}{2i}\int d^2q\, e^{2i(p_\theta q_\theta+p_\phi q_\phi)}\partial_{q_\theta} \times[\Theta(\theta_-,\phi_-)\ \Theta^*(\theta_+,\phi_+)],$$

$$p_\theta\partial_{p_\theta}\rho(\theta,\phi,p_\theta,p_\phi)=-\int d^2q\, e^{2i(p_\theta q_\theta+p_\phi q_\phi)}\partial_{q_\theta} \times[q_\theta\ \Theta(\theta_-,\phi_-)\ \Theta^*(\theta_+,\phi_+)]$$

one obtains, after lengthy simplifications, the result that the stationary solutions of the Liouville equation (14) satisfy

$$\frac{i}{2\pi^2}\int d^2q\, e^{2i(p_\theta q_\theta+p_\phi q_\phi)}\frac{1}{r^2+q^2}\left(f_1+\frac{1}{r}f_2\right)=0, \tag{16}$$

where

$$\begin{aligned}f_1={}&\Theta^*\left[\frac{1}{\sin\theta_-}\partial_{\theta_-}(\sin\theta_-\ \partial_{\theta_-}\Theta)+\frac{1}{\sin^2\theta_-}\partial^2_{\phi_-}\Theta\right]\\&-\Theta\left[\frac{1}{\sin\theta_+}\partial_{\theta_+}(\sin\theta_+\partial_{\theta_+}\Theta^*)+\frac{1}{\sin^2\theta_+}\partial^2_{\phi+}\Theta^*\right],\end{aligned}$$

$$\begin{aligned}f_2={}&-\frac{q^2}{2r}(\cos\theta_++\cos\theta_-)\left(\frac{\Theta^*\partial_{\theta_-}\Theta}{\sin\theta_-}-\frac{\Theta\partial_{\theta_+}\Theta^*}{\sin\theta_+}\right)\\&-\frac{r}{2}(\cos\theta_+-\cos\theta_-)\left(\frac{\Theta^*\partial_{\theta_-}\Theta}{\sin\theta_-}+\frac{\Theta\partial_{\theta_+}\Theta^*}{\sin\theta_+}\right)\\&+q_\phi\sin\theta\left(\frac{\Theta^*\partial_{\phi_-}\Theta}{\sin^2\theta_-}+\frac{\Theta\partial_{\phi_+}\Theta^*}{\sin^2\theta_+}\right),\end{aligned}$$

and $q^2=q^2_\theta+q^2_\phi$. It is implied that Θ is a function of the variables θ_- and ϕ_- while Θ^* is a function of θ_+ and ϕ_+.

If the function f_2 is neglected for the moment then the condition (16) implies that the angular function satisfies the differential equation

$$\frac{1}{\sin\theta}\partial_\theta(\sin\theta\partial_\theta\Theta)+\frac{1}{\sin^2\theta}\partial^2_\phi\Theta=\lambda\Theta,$$

where λ is a real constant. In this equation one recognizes the equation for spherical harmonics, where $\lambda=-l(l+1)$. However, the function f_2 cannot be neglected, and therefore the angular functions are only approximately the spherical harmonics. However, a very useful feature of the function f_2 is that in the limits $q_\theta\to0$ and $q_\phi\to0$ it is equal to zero, in which case the angular functions are exactly the spherical harmonics. This means that when the phase space density is integrated over the momentum variables the resulting probability density should be the squared modulus of the spherical harmonics, i.e.,

$$\begin{aligned}P(\theta,\phi)&=\int dp_\theta\int dp_\phi\,\rho(\theta,\phi,p_\theta,p_\phi)\\&=|\Theta(\theta,\phi)|^2=|Y_{l,m}(\theta,\phi)|^2.\end{aligned} \tag{17}$$

The choice of the spherical harmonics for the angular functions means that the phase space density is approximate, which is manifested as being time dependent, i.e., it is not a function of only the dynamic invariants of the rigid rotor. This is the price that is paid for neglecting the function f_2 in Eq. (16). Inclusion of this function results in the phase space density that is a function of only these invariants, and this fact is used as the procedure to find a proper phase space density. This is best demonstrated by one example. One particular case, however, has an exact solution, and this is when the angular function is constant. In this case

$$\begin{aligned}\rho_{0,0}(\theta,\phi,p_\theta,p_\phi)&=\frac{1}{\pi^2}\int d^2q\, e^{2i(p_\theta q_\theta+p_\phi q_\phi)}\frac{1}{4\pi}\\&=\frac{1}{4\pi}\delta(p_\theta)\delta(p_\phi).\end{aligned}$$

The example that will be analyzed in more detail is when the angular function is the spherical harmonic $Y_{1,0}(\theta,\phi)$. The phase space density (15) is

$$\rho(\theta,\phi,p_\theta,p_\phi,t)=\frac{1}{\pi^2}\int d^2q\, e^{2i(p_\theta q_\theta+p_\phi q_\phi)} \times Y^*_{1,0}(\theta_+,\phi_+)Y_{1,0}(\theta_-,\phi_-)$$

and its explicit form is (the constant r is fixed to unity)

$$\begin{aligned}\rho(\theta,\phi,p_\theta,p_\phi,t)\\={}&\frac{3}{4\pi^3}\int d^2q\, e^{2i(p_\theta q_\theta+p_\phi q_\phi)}\frac{q^2_\theta\sin^2\theta-\cos^2\theta}{1+q^2}\\={}&\frac{3}{2\pi^2}\left(1-\frac{p^2_\phi\sin^2\theta}{p^2}\right)K_0(2p)+\frac{3\sin^2\theta}{4p\pi^2}\\&\times\left(1-2\frac{p^2_\phi}{p^2}\right)K_1(2p)-\frac{3}{8\pi}\delta(p_\theta)\delta(p_\phi)\sin^2\theta\end{aligned}$$

where $K_n(x)$ is a modified Bessel function of the second kind. This phase space density is not stationary, because the term

$$\rho_t=\frac{3\sin^2\theta}{4p\pi^2}K_1(2p)$$

is not a combination of dynamic invariants. However, if p_ϕ is replaced by $p\cos\alpha$ then

$$\int_0^{2\pi}d\alpha\left(1-2\frac{p_\phi^2}{p^2}\right)=0,$$

which means that these two terms in the phase space density can be omitted without in any way modifying the integral (17), the value of the total angular momentum squared

$$\langle L^2\rangle=\int d\Omega\int d^2p\,p^2\rho(\theta,\phi,p_\theta,p_\phi),$$

on the angular momentum (its zth component)

$$\langle\vec{L}\rangle=\hat{z}\int d\Omega\int d^2p\,p_\phi\sin\theta\rho(\theta,\phi,p_\theta,p_\phi)=\langle L_z\rangle\hat{z}.$$

Therefore,

$$\rho_{1,0}(\theta,\phi,p_\theta,p_\phi)=\frac{3}{2\pi^2}\left(1-\frac{p_\phi^2\sin^2\theta}{p^2}\right)K_0(2p)-\frac{3}{8\pi}\delta(p_\theta)\delta(p_\phi)\sin^2\theta$$

is time independent and represents the phase space density for a rigid rotor in the state with angular momentum squared $\langle L^2\rangle=2$ and angular momentum $\langle L_z\rangle=0$, while the probability density (17) is $P(\theta,\phi)=|Y_{1,0}(\theta,\phi)|^2$. Similarly, the phase space density for $l=1$ and $m=1$ is

$$\rho_{1,1}(\theta,\phi,p_\theta,p_\phi)=\frac{3}{4\pi^2}\left(1+\frac{p_\phi^2\sin^2\theta}{p^2}\right)K_0(2p)+\frac{3p_\phi\sin\theta}{2\pi^2p}K_1(2p)+\frac{3}{16\pi}\times(-2+\sin^2\theta)\delta(p_\theta)\delta(p_\phi)$$

with the property that $P(\theta,\phi)=|Y_{1,1}(\theta,\phi)|^2$, $\langle L^2\rangle=2$, and $\langle L_z\rangle=1$.

The phase space densities for the angular momentum states $(2,m)$, $m=0,1,2$, were calculated as additional examples. They are associated with the angular momentum squared value $\langle L^2\rangle=6$ and the angular momentum $\langle L_z\rangle=0,1,2$, respectively. They are

$$\rho_{2,0}(\theta,\phi,p_\theta,p_\phi)=\frac{15}{4\pi^2}\left(-1+\frac{p_\phi^4\sin^4\theta}{p^4}\right)K_0(2p)+\frac{45p}{8\pi^2}\times\left(1-\frac{p_\phi^2\sin^2\theta}{p^2}\right)^2K_1(2p)+\frac{5}{128\pi}\times(8-24\sin^2\theta+27\sin^4\theta)\delta(p_\theta)\delta(p_\phi),$$

$$\rho_{2,1}(\theta,\phi,p_\theta,p_\phi)=\frac{15}{4\pi^2}\left(-1+2p_\phi\sin\theta+\frac{p_\phi^2\sin^2\theta}{p^2}-2p_\phi^3\sin^3\theta-\frac{2p_\phi^4\sin^4\theta}{3p^4}\right)K_0(2p)+\frac{15p}{4\pi^2}\left(1-2\frac{p_\phi^3\sin^3\theta}{p^4}-\frac{p_\phi^4\sin^4\theta}{p^4}\right)\times K_1(2p)+\frac{15}{16\pi}\left(\sin^2\theta-\frac{3}{4}\sin^4\theta\right)\times\delta(p_\theta)\delta(p_\phi),$$

$$\rho_{2,2}(\theta,\phi,p_\theta,p_\phi)=\frac{15}{8\pi^2}\left(-1+2p_\phi\sin\theta-2\frac{p_\phi^2\sin^2\theta}{p^2}+2\frac{p_\phi^3\sin^3\theta}{p^2}+\frac{p_\phi^4\sin^4\theta}{3p^4}\right)K_0(2p)+\frac{15p}{16\pi^2}\left(1-4\frac{p_\phi\sin\theta}{p^2}+6\frac{p_\phi^2\sin^2\theta}{p^2}+\frac{4p_\phi^3\sin^3\theta}{3p^4}+\frac{p_\phi^4\sin^4\theta}{p^4}\right)K_1(2p)+\frac{15}{32\pi}\left(1-\sin^2\theta+\frac{3}{8}\sin^4\theta\right)\delta(p_\theta)\delta(p_\phi).$$

In this way the phase space for the true rigid rotor can be defined. It is "true" because only the variables that are relevant for such an object were introduced.

V. DISCUSSION

Angular momentum in phase space was analyzed, and in this context the rigid rotor was discussed. Perhaps one of the most intriguing findings is the interpretation of the partition of the kinetic energy operator, which is in considerable disagreement with the standard one. Part of what is considered to be radial kinetic energy is in fact a contribution from the angular momentum operator, despite the fact that it contains only radial variables. This finding does not come as a surprise if one makes the following observation in traditional classical mechanics. Given spherically symmetric probability distributions of coordinates $P(r)$ and momenta $Q(p)$ for a free particle (say, obtained by measuring its position and momentum) the average kinetic energy is not zero despite the fact that the momentum is. Likewise, the average angular momentum is zero but its average modulus squared is not because

$$\langle L^2\rangle = \int d^3r \int d^3p\, r^2(p_\theta^2+p_\phi^2)P(r)Q(p)\neq 0.$$

Introducing the uncertainty principle does not change this fact, except that instead of this average having an arbitrary value it is fixed and equal to 3/2. Therefore a particle always has a nonzero modulus of angular momentum, and its minimal value is fixed and independent of the phase space density. This is like saying that the particle always carries a minimal intrinsic angular momentum, but in the way it is described it never manifests itself. For all practical purposes this finding is immaterial, because the standard interpretation is self-sufficient, but it becomes evident when classical modeling is attempted.

From the phase space density for the rigid rotor one expects to obtain the momentum space probability density, which is given by

$$Q(\vec{p}) = \int d^3r\, \rho(\vec{r},\vec{p}).$$

However, one should be careful about the components of the momentum variable. Throughout this paper the components with respect to the vector $\vec{r}$ were used, because they are natural when angular momentum is analyzed. This is because p_θ and p_ϕ are components along the appropriate angular unit vectors that are perpendicular to the vector $\vec{r}$ and hence directly proportional to the angular momentum (they can be called the radius vector components of the momentum). However, in momentum space one works only with the components of the momentum vector, for which this is not the case. If p is the modulus of the vector $\vec{p}$ while θ_p and ϕ_p are its spherical angles, then

$$\begin{aligned} p_r &= p(\cos\theta\cos\theta_p+\cos[\phi-\phi_p]\sin\theta\sin\theta_p), \qquad (18)\\ p_\theta &= p(\sin\theta\cos\theta_p-\cos[\phi-\phi_p]\cos\theta\sin\theta_p),\\ p_\phi &= -p\sin[\phi-\phi_p]\sin\theta_p, \end{aligned}$$

which explicitly shows that the radius vector components of momentum are a mixture of momentum and radial vector spherical coordinates. Therefore in the phase space density they must be replaced by Eq. (18) and integration over the spatial coordinates performed. Indeed, for the "soft" rigid rotor it can be shown that one obtains for the momentum distribution the square modulus of Eq. (11), but it is not clear what the outcome would be for the true rigid rotor. For the latter it is required that $p_r=0$ and yet the expression for the phase space density would be a function of p and θ_p without an obvious restriction of that kind. However, the explicit expression for the momentum probability is not of importance; it is only important to be able to calculate the averages. For example, the average of the square of the Cartesian component p_x, say, with the phase space density $\rho_{2,0}$, is given by

$$\begin{aligned} \langle p_x^2\rangle &= \int d\Omega\, dp_\theta\, dp_\phi [p_\phi\sin\phi+p_\theta\cos\theta\cos\phi]^2\\ &\quad\times\rho_{2,0}(\theta,\phi,p_\theta,p_\phi)\\ &= \frac{22\pi}{7}, \end{aligned}$$

where we set $p_r=0$.

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[1] See any standard textbook on angular momentum, e.g., R. N. Zare, *Angular Momentum* (Wiley, New York, 1988).

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