ON THE MOMENT OF INERTIA OF A MANY-PARTICLE SYSTEM; I.

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The problem of the determination of the moment of inertia is considered. The formula obtained has as the simplest consequence that, even in the case of a spherically symmetric system, the moment of inertia is different from zero, and is not even very small as compared to the moment of inertia of a rigid body.

THE problem of the determination of the moment of inertia has been considered in a number of papers[1-3] (a more detailed bibliography is given in a paper by Bohr and Mottelson,[3] which is soon to appear). However, as far as we know, a sufficiently general expression for the operator of the moment of inertia has so far not been given. One of the aims of the present paper is to fill this gap to some extent by investigating the problem of the determination of the moment of inertia of a system rotating about a fixed axis.

We also discuss some estimates for the lower limit of the possible values of the moment of inertia. One of these estimates leads to the result that the moment of inertia of a spherically symmetric system (we mainly have in mind the spherically symmetric nucleus) is not only different from zero, as is frequently assumed, but is not even very small as compared to the momentum of inertia of a rigid body.

1. THE COLLECTIVE ANGLE VARIABLE φ

We shall attempt to develop the theory in a form which is independent of the specific method of separation of the collective angular variable. The separation itself is, however, a necessary feature of the theory. It may be achieved in the following manner.

Suppose we have a system of N particles with, in general, different masses. The Hamiltonian of the system is equal to

$$H = \sum^{N} (\hbar^2/2m)(\partial^2/\partial x^2 + \partial^2/\partial y^2 + \partial^2/\partial z^2) + U. \qquad (1)$$

The summation in (1) goes over all particles; the particle indices are omitted.

We assume that the potential U is independent of the velocity and commutes with the operator corresponding to the projection of the total angular momentum on the axis of rotation, which we choose as the z axis. We use the notation $M_z \equiv M$, where

$$M = \sum^{N} - i\hbar (x\partial/\partial y - y\partial/\partial x). \qquad (2)$$

Then

$$[H, M] = 0. \qquad (3)$$

We introduce a certain operator φ, which depends only on the coordinates x and y and satisfies the condition

$$[M, \varphi] = - i\hbar. \qquad (4)$$

With the help of the equations

$$(i/\hbar)[H, \varphi] = -V + M/\hat{I}_0, \quad -\hbar^{-2}[[H, \varphi], \varphi] = 1/\hat{I}_0 \qquad (5)$$

we also introduce the operators V and $\hat{I}_0$. Written more explicitly, these operators have the form

$$\frac{1}{\hat{I}_0} = \sum^{N} \frac{1}{m}\left[\left(\frac{\partial\varphi}{\partial x}\right)^2 + \left(\frac{\partial\varphi}{\partial y}\right)^2\right],$$

$$V = \sum - i\hbar\left[\frac{1}{\hat{I}_0}\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right) - \frac{1}{m}\left(\frac{\partial\varphi}{\partial x}\frac{\partial}{\partial x} + \frac{\partial\varphi}{\partial y}\frac{\partial}{\partial y}\right) - \frac{1}{2m}\left(\frac{\partial^2\varphi}{\partial x^2} + \frac{\partial^2\varphi}{\partial y^2}\right)\right]. \qquad (6)$$

It follows from equations (3) and (4) that the operators $\hat{I}_0$ and V commute with φ and M. The same obviously holds for the operator H′ defined by

$$H = H' - VM + M^2/2\hat{I}_0. \qquad (7)$$

The quantity φ can always be regarded as a new independent variable, by choosing the remaining $3N-1$ variables ξ such that

$$[M, \xi] = 0 \qquad (8)$$

for all ξ. The operator M then has the form

$$M = -i\hbar\partial/\partial\varphi,$$

and the operators H', $\hat{I}_0$, and V are functions of ξ and $\partial/\partial\xi$ only.

The new variable φ can be interpreted as the angle of rotation of the system as a whole (for more detail, cf. Sec. 3). Correspondingly, the variables ξ have the meaning of internal coordinates. The operator H' represents the energy of internal motion. The operator VM represents the energy of interaction of the internal motion with the rotation.

2. MOMENT OF INERTIA

We introduce the complete system of eigenfunctions of the operators H and M:

$$H\Psi_n = E_n\Psi_n; \qquad M\Psi_n = M_n\Psi_n. \tag{9}$$

The functions belonging to the eigenvalue $M_n = 0$ will be denoted by Φ_n.

We consider an initial state Ψ_0 with eigenvalues E_0 and M_0. We may write

$$\Psi_0 = (2\pi)^{-1/2} \exp\left\{\frac{i}{\hbar} M\varphi\right\} \Psi_0', \tag{10}$$

where Ψ_0' is a function depending only on the internal variables ξ. By operating on Ψ_0 with the Hamiltonian (7) we obtain

$$(H' - VM_0 + M_0^2/2\hat{I}_0)\Psi_0' = E_0\Psi_0', \qquad \text{with } M\Psi_0' = 0. \tag{11}$$

Equation (11) is initially obtained for integral values of $M_0/\hbar$. It remains, however, meaningful for arbitrary values of $M_0/\hbar$. It then determines E_0 as a function of some continuous parameter M_0. We assume that, for not too large M_0, this function can be expanded in powers of M_0:

$$E_0(M_0) = E_0(0) + M_0^2/2I + \ldots \tag{12}$$

One easily sees that the absence of the odd powers of M_0 in expansion (12) is connected with the equivalence of the right and left handed systems of coordinates.

The expansion (12) can be terminated after the quadratic term in M_0. In this case we talk about a purely rotational spectrum. In the presence of higher terms in the expansion, the rotational spectrum will be more or less modified. Nevertheless, in both cases, the quantity I should obviously be interpreted as a moment of inertia. The reciprocal quantity

$$B = 1/I \tag{13}$$

is naturally called the inverse moment of inertia. It follows from (12) that

$$B = (\partial^2 E_0/\partial M_0^2)_{M_0=0}. \tag{14}$$

We note that the expansion (12) is formally just the usual perturbation series for the case that M_0 is a small parameter. The coefficients of this series are well known. In particular, we obtain the coefficient (14) by applying the operator $1/\hat{I}_0$ once and the operator V twice. As a result, we obtain

$$\frac{1}{I} = \left\langle \Phi_0, \frac{1}{\hat{I}_0}\Phi_0 \right\rangle - 2\sum_{n\neq 0}\frac{1}{E_n - E_0}|\langle\Phi_n, V\Phi_0\rangle|. \tag{15}$$

This is the required expression for the moment of intertia for the case of rotation about a fixed axis z.

In operator form we have

$$\frac{1}{\hat{I}} = \frac{1}{\hat{I}_0} - 2V\mathrm{P}\frac{1}{H' - E_0}V, \tag{16}$$

where P denotes the principal value. The operator $1/\hat{I}$ may be written in a more convenient form by assuming the existence of an operator Λ satisfying the condition

$$V = (i/\hbar)[H', \Lambda], \tag{17}$$

where

$$V_{0n} = (-i/\hbar)(E_n - E_0)\Lambda_{0n}, \qquad V_{n0} = (i/\hbar)(E_n - E_0)\Lambda_{n0}.$$

In this case we may write

$$2\sum_{n\neq 0}\frac{|V_{n,0}|^2}{E_n - E_0} = \frac{i}{\hbar}\sum_n (V_{0n}\Lambda_{n0} - \Lambda_{0n}V_{n0}) = \frac{i}{\hbar}[V, \Lambda]_{00},$$

and therefore

$$1/\hat{I} = 1/\hat{I}_0 - (i/\hbar)[V, \Lambda]. \tag{18}$$

As an example we consider the problem of two interacting two-dimensional rigid rotators, each of which is characterized by its constant moment of inertia μ_i ($i = 1, 2, \ldots, N$).

The Hamiltonian of this system is

$$H = \sum_{i=1}^{N}(-\hbar^2/2\mu_i)\,\partial^2/\partial\varphi_i^2 + U. \tag{19}$$

φ_i is the angular coordinate of the i-th rotator.

It is entirely obvious that, by choosing the collective angular variable φ in the form

$$\varphi = \sum_{i=1}^{N}\mu_i\varphi_i \Big/ \sum_{i=1}^{N}\mu_i, \tag{20}$$

we achieve a complete separation of the internal and external motions ($V = 0$!). The moment of inertia is equal to

$$I = \hat{I}_0 = \sum_{i=1}^{N}\mu_i. \tag{21}$$

We are, however, interested in the case when φ is chosen such that the operator V is different from zero. We then have to use the general formulas (15) or (18) for the determination of the moment of inertia. In particular, we assume that $\varphi = \varphi_1$; then

$$\hat{I}_0 = \mu_1;\quad V = \frac{1}{\mu_1}\sum_{i=2}^{N} - i\hbar\frac{\partial}{\partial\varphi_i};\quad \Lambda = \frac{1}{I}\sum_{i=2}^{N}\mu_i(\varphi_i - \varphi). \quad (22)$$

Substituting the operators (22) in formula (18) we again obtain the correct value (20) for the moment of inertia. In the given special case it is thus possible to verify explicitly the independence of the moment of inertia of the choice of φ. This independence corresponds to the fact that the moment of inertia is determined by observable quantities (the energy and the projection of the angular momentum on the axis of rotation), which are, of course, invariant under arbitrary coordinate transformations.

3. ANGULAR VELOCITY OF THE SYSTEM AS A WHOLE

The inverse moment of inertia can also be determined as the derivative of the angular velocity with respect to the projection of the angular momentum on the axis of rotation z. The meaning of the angular velocity of the system is, however, not completely obvious. In this connection it is of interest to investigate the reverse problem: the determination of the angular velocity as that quantity which, upon differentiation with respect to M_0, gives the correct expression for the inverse moment of inertia. It is easily seen that the following quantity has this property:

$$\Omega = \langle \Psi'_0, \dot{\varphi}\Psi'_0 \rangle, \quad (23)$$

where the dot above the operator denotes the commutator with the Hamiltonian multiplied by $i/\hbar$.

Indeed, we have, according to formula (11),

$$\left(\frac{\partial \Psi'_0}{\partial M_0}\right)_{M_0=0} = \mathrm{P}\frac{1}{H' - E_0}V\Phi_0. \quad (24)$$

Furthermore,

$$\dot{\varphi}\Psi'_0 = \left(-V + \frac{M_0}{\hat{I}_0}\right)\Psi'_0, \quad (25)$$

hence

$$\left\{\frac{\partial}{\partial M_0}\left[\left(-V + \frac{M_0}{\hat{I}_0}\right)\Psi'_0\right]\right\}_{M_0=0} = \frac{1}{\hat{I}_0}\Phi_0 - V\left(\frac{\partial \Psi'_0}{\partial M_0}\right)_{M_0=0}, \quad (26)$$

and, finally,

$$\left(\frac{\partial \Omega}{\partial M_0}\right)_{M_0=0} = \left\langle \Phi_0, \frac{1}{\hat{I}_0}\Phi_0\right\rangle - 2\left\langle \Phi_0, V\mathrm{P}\frac{1}{H' - E_0}V\Phi_0\right\rangle.$$

This is exactly formula (15).

We can easily determine the angular acceleration by expanding expression (23) for the angular velocity of the system. It may also be used for the determination of the moment of inertia. We again obtain, of course, the same result (15) as before.

4. ESTIMATE OF THE LOWER LIMIT OF THE MOMENT OF INERTIA

Expression (15) for the inverse moment of inertia consists of two structurally different terms. The first term,

$$\frac{1}{I_0} = \left\langle \Phi_0, \frac{1}{\hat{I}_0}\Phi_0\right\rangle, \quad (27)$$

defines some "bare" moment I_0, which plays the role of a generalized "bare" mass corresponding to the generalized coordinate φ. The second term represents a correction to the "bare" moment due to the coupling between the separate particles of the system during the rotation. It is immediately clear from formula (15) that, at least for the ground state of the system, the "bare" moment of inertia is always smaller than the true moment:

$$I_0 < I. \quad (28)$$

The "bare" moment therefore represents a lower limit for the possible values of the total moment. In this connection it is very desirable to find that φ for which the "bare" moment has the largest value. The case mostly considered in the literature so far is that in which φ represents the angle of rotation of the principal axes of the system (see, e.g., reference 2). In this case the operator $\hat{I}_0$ represents the so-called hydrodynamic moment of inertia

$$\hat{I}_0 = \left\{\left[\sum^{N} m(x^2 - y^2)\right]^2 + \left[\sum^{N} 2mxy\right]^2\right\} \Big/ \sum^{N} m(x^2 + y^2).$$

It is an interesting fact that, after averaging over a spherically symmetrical distribution, this quantity takes on a nonvanishing, if small, value.

By choosing φ in the form

$$\varphi = \sum_{i=1}^{N} m_i\rho_i^2\varphi_i \Big/ \sum_{i=1}^{N} m_i\rho_i^2, \quad (29)$$

where ρ_i and φ_i are the cylindrical coordinates of the i-th particle, and $\rho_i = (x_i^2 + y_i^2)^{1/2}$, we may convince ourselves that even in the completely symmetrical case the moment of inertia is not only different from zero, but is not even very small in comparison to the moment of inertia of a rigid body. Indeed, we then obtain the following expression for $\hat{I}_0$:

$$\hat{I}_0 = \sum_{i=1}^{N} m_i\rho_i^2 \Big/ \left\{1 + 4\sum_{i=1}^{N} m_i\rho_i^2(\varphi_i - \varphi)^2 \Big/ \sum_{i=1}^{N} m_i\rho_i^2\right\}. \quad (30)$$

The quantity $(\varphi_i - \varphi)^2$ may be replaced by its average value

$$\overline{(\varphi_i - \varphi)^2} = \pi^2/3$$

and can then be taken outside the summation sign. This yields

$$\hat{I}_0 \approx \sum_{i=1}^{N} m_i\rho_i^2 \Big/ \left(1 + \frac{4\pi^2}{3}\right) \approx \frac{1}{14}\sum_{i=1}^{N} m_i\rho_i^2. \quad (31)$$

The moment of inertia of the ground state can therefore not be smaller than $1/14$ of the moment of inertia of a rigid body.

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