

Relation between the moment of inertia and moments of density

M. Rosina

*Faculty of Natural Sciences and Technology, University of Ljubljana and J. Stefan Institute,
Jadranska 19, POB.64, SI-61111 Ljubljana, Slovenia*

P. Van Leuven

*Department of Mathematics and Computer Science, University of Antwerp, Rijksuniversitair Centrum Antwerpen,
Groenenborgerlaan 171, B2020 Antwerpen, Belgium*

(Received 29 July 1992; revised manuscript received 16 July 1993)

The moment of inertia of a physical system exhibiting irrotational flow is expressed as a series expansion in terms of the moments of the density distribution. The lowest-order contribution yields a simple relation with the quadrupole moment and is applicable to models of classical and quantum systems. The method is applied in some detail to the special case of the rotational magnetic moment of the hydrogen molecule.

PACS number(s): 03.65. — w, 33.10.Ev

I. INTRODUCTION

Rotation is a type of motion occurring in many fields of physics, both classical and quantal. Although the underlying dynamics can be very different, the kinematics of rotational motion is usually described by means of the moment of inertia \mathcal{J} which is defined as the ratio of the angular momentum L to the angular velocity ω . For quantum systems it is impossible to give a general definition of the angular velocity as an observable but there are several situations in which this concept is clearly defined through the idea of "cranking." In that method one thinks, for example, of particles in a deformed potential well that is rotated by some cranking mechanism. In nuclear physics, the Inglis model assumes a deformed, rotating self-consistent mean field for the particles and this looks very much like an externally cranked potential. In molecular physics, the rotating nuclei provide a cranked field for the electrons. In all these cases one can easily derive a formula for the moment of inertia. It has the form

$$\mathcal{J} = 2 \sum_n \frac{|\langle 0 | L_x | n \rangle|^2}{E_n - E_0} \quad (1)$$

and is referred to as Inglis's formula in nuclear physics [1] or "Wick's formula" in molecular physics [2]. This formula necessitates the knowledge of all excited states $|n\rangle$ for the calculation of the moment of inertia of the ground state $|0\rangle$.

It is the objective of this paper to present an expression of the moment of inertia which is more practical because it needs information about the ground state only. Moreover, it is conceptually more general as it can also be applied to classical fluid dynamics. We restrict our investigation to cases of irrotational flow, which in the case of classical systems is, in a way, the simplest assumption and is realistic for many situations in nonviscous fluids. For quantal systems it is well known that for a single particle, or for many particles all occupying the same single-

particle state, the velocity field (of probability) is irrotational. We shall show that in this case the moment of inertia is expressible as an expansion in multipole moments of the ground-state density distribution

$$\mathcal{J} = \sum_{i,j} Q_i M_{i,j}^{-1} Q_j \quad (2)$$

with definitions of Q and M to be given below.

In Sec. II we shall give the necessary definitions in terms of an essentially hydrodynamical formulation. In Sec. III we describe the central idea of our method and in Sec. IV we discuss the first approximation of the series expansion obtained in Sec. III. We illustrate the formula on the example of the rotational gyromagnetic factor of the hydrogen molecule. It should be stressed here that we do not endeavor to reproduce the highly sophisticated calculations [3] but only want to show that one can obtain a very reliable result on the basis of a simple theory.

II. VELOCITY FIELD OF A CRANKED PARTICLE

The basic objective of the cranking model is to determine the inertial parameters of the collective motion (*in casu* the moment of inertia for rotation) of a quantum system from its response to an external force (*in casu* the Coriolis force). We shall describe here the motion of a single particle in a cranked nonspherical potential. The derivation is equally valid for a many-body system if all particles occupy the same single-particle state, as is the case in the ground state of bosonic systems such as superfluid helium or as it is approximately true for the two electrons in the hydrogen molecular ground state.

For definiteness, we consider a single particle with mass m and charge e and choose the x axis as the rotation axis. If the potential in the absence of cranking is $V(\mathbf{r})$ and we apply a uniform rotational cranking with angular velocity ω , then the problem is that of a particle in an explicit time-dependent field $\exp(-i\omega\hat{l}_x) V(\mathbf{r}) \exp(i\omega\hat{l}_x)$, where \hat{l}_x is the x component of the angular momentum.

It is convenient to solve it in the "body system" which rotates together with the cranked potential because there the ground state is stationary. In the body system the Hamiltonian reads

$$H_\omega = -\frac{\hbar^2}{2m}\Delta + V(\mathbf{r}) - \omega\hat{L}_x. \quad (3)$$

For the description of the ground-state properties it is convenient to use the density field $\rho(\mathbf{r})$ and the phase field $\phi(\mathbf{r})$ instead of the wave function ψ . The relation is (in the laboratory system)

$$\psi = \sqrt{\rho} \exp\left[\frac{im}{\hbar}\phi\right]. \quad (4)$$

It is also useful to introduce the current field

$$\mathbf{j} = \frac{i\hbar}{2m}(\psi\nabla\psi^\dagger - \psi^\dagger\nabla\psi), \quad (5)$$

which obeys the continuity equation

$$\text{div}\mathbf{j} + \frac{\partial\rho}{\partial t} = 0. \quad (6)$$

In the laboratory system the velocity field \mathbf{j}/ρ is irrotational, while in the body system it has constant rotor and is given by¹

$$\mathbf{v}(\mathbf{r}) = \nabla\phi(\mathbf{r}) - \omega \times \mathbf{r}. \quad (7)$$

It is legitimate to call ϕ the velocity potential. The continuity equation, the equation $\nabla \times \mathbf{v} = -2\omega$ [which follows from (7)], and the boundary condition that currents vanish rapidly enough toward infinity give a unique solution for \mathbf{j} if ρ is known. Therefore we need only the knowledge of the density field in order to determine the current field and all the observables. We determine ϕ from ρ by solving the continuity equation

$$\rho\Delta\phi + (\nabla\rho) \cdot (\nabla\phi) - (\nabla\rho) \cdot (\omega \times \mathbf{r}) = 0. \quad (8)$$

We assume that ω is small enough that the density does not change much with ω and we can take the nonrotating ground-state value. As a first-order perturbation, the cranking introduces $\mathbf{j} \neq 0$ but does not change ρ yet. This assumption can be verified experimentally by observing that corresponding observables do not change much with increasing rotational angular momentum.

We shall be interested in the "average" angular momentum in the x direction $L_x = \langle \psi | \hat{L}_x | \psi \rangle$. It is proportional to ω because the driving term in the continuity equation is proportional to ω . Therefore we can introduce the moment of inertia by the relation

$$\mathcal{J} = \frac{1}{m\omega} L_x. \quad (9)$$

It can be expressed in terms of the density and the velocity potential (see Appendix A)

$$\mathcal{J} = \frac{1}{\omega} \mathbf{e}_x \cdot \int (\mathbf{r} \times \nabla\phi) \rho d^3r. \quad (10)$$

We note here that the quantity thus defined has the dimension of $[length]^2$; it is the specific moment of inertia per unit of mass. The usual inertial moment of the mass flow is $m\mathcal{J}$.

III. EXPANSION IN MOMENTS OF DENSITY

In the previous section we have shown that the probability density of a cranked particle in its ground state carries all the information needed to calculate observables. In the present section we show how the moment of inertia can be expanded in moments of the density distribution. The derivation yields a simple formula for the leading term and an easy algorithm for higher terms. The condition for the expansion is that the velocity potential field ϕ is analytic in the region of nonvanishing density and can be expanded in a polynomial of \mathbf{r} . The approach consists of taking in the definition of the moment of inertia (10) as input the exact ρ and an approximate \mathbf{v} . The "ansatz" for \mathbf{v} is fitted so as to satisfy the continuity equation (8) up to a certain order (see below).

In this section we restrict ourselves to systems where there is no (or negligible) flow parallel to the cranking axis. Then the continuity equation is satisfied separately for each x value and the moment of inertia is a sum of separate contributions from each x . It is therefore sufficient to describe the two-dimensional problem in the (y, z) coordinates. The generalization to the three-dimensional problem is straightforward.

Our ansatz for the velocity potential will be a polynomial of order N ($\mu + \nu \leq N$):

$$\phi(y, z) = \omega \sum_{\mu, \nu} A_{\mu\nu} y^\mu z^\nu. \quad (11)$$

We introduce the moments of the density

$$R_{\mu, \nu} = \int \rho(y, z) y^\mu z^\nu dy dz. \quad (12)$$

In general, the continuity equation cannot be solved exactly for a finite order N . The best we can do is to write moments of the continuity equation to order N and then solve a coupled system of linear equations with the same number of equations as unknowns. From (8) follows (upon multiplication by $y^{\mu'} z^{\nu'}$ and integration over y and z)

$$\sum_{\mu, \nu} M_{\mu'\nu', \mu\nu} A_{\mu\nu} = Q_{\mu'\nu'}, \quad (13)$$

where we have introduced the modified moments

$$M_{\mu'\nu', \mu\nu} = \mu' \mu R_{\mu'-2+\mu, \nu'+\nu} + \nu' \nu R_{\mu'+\mu, \nu'-2+\nu}, \quad (14)$$

$$Q_{\mu\nu} = \nu R_{\mu+1, \nu-1} - \mu R_{\mu-1, \nu+1}. \quad (15)$$

The moment of inertia can now simply be written in the form

$$\mathcal{J} = \sum_{\mu, \nu} A_{\mu\nu} Q_{\mu\nu}, \quad (16)$$

where the coefficients $A_{\mu\nu}$ are determined from the linear

¹In the following the symbols ρ , \mathbf{j} , and \mathbf{v} refer to the body system.

equations (13). We can also write

$$\mathcal{J} = \sum_{\mu, \nu, \mu', \nu'} Q_{\mu\nu} M_{\mu\nu, \mu'\nu'}^{-1} Q_{\mu'\nu'} \quad (17)$$

which is precisely the formula (2) announced in the Introduction. We note that in (13) the monopole terms are absent, consistent with the fact that the constant term in ϕ is irrelevant. Without loss of generality we can choose the cranking axis through the centroid of ρ such that also the dipole terms vanish. Hence, the leading contribution in (13) comes from the quadrupole terms $N=2$. If one supposes furthermore that ρ has reflection symmetry with respect to the planes $y=0$ and $z=0$, all $R_{\mu, \nu}$ with odd values of μ or ν vanish and consequently only equations with even N subsist. In that case the next but leading term in (13) is the hexadecapole $N=4$.

IV. QUADRUPOLE FORMULA

If we restrict the expressions of the previous section to the leading quadrupole terms, we obtain a set of three equations for A_{20} , A_{11} , and A_{02} . Without loss of generality we can choose the y and z axes as principal axes of the quadrupole tensor. Then it follows that A_{20} and A_{02} are both zero and we find $A_{11} = (R_{20} - R_{02}) / (R_{20} + R_{02})$. The corresponding expression for the moment of inertia is then

$$\mathcal{J} = \frac{Q^2}{M} \quad (18)$$

where we have put

$$Q = Q_{11} = \int (y^2 - z^2) \rho d^3r \quad (19)$$

$$M = M_{11,11} = \int (y^2 + z^2) \rho d^3r \quad (20)$$

Formula (18) relates the moment of inertia to the quadrupole moment and the mean-square radius.

Now the interesting question arises: for which ρ is the expression (18) exact? We first note that because ϕ contains only the term $A_{11}yz$ its Laplacian is zero. Therefore the continuity equation (8) reduces to

$$\nabla \rho \cdot (\nabla \phi - \omega \times \mathbf{r}) = \nabla \rho \cdot \mathbf{v} = 0 \quad (21)$$

This expresses the fact that the equidensity lines coincide with the flow lines of the velocity field. We can conclude, more generally, that "a sufficient condition for a divergenceless velocity field to solve the continuity equation is that its flow lines coincide with the equidensity lines."

In our present case (where ϕ contains only the A_{11} term) the flow lines in the body system are conformal ellipses with half axes squared proportional to R_{20} and R_{02} ; therefore the density may be of the form

$$\rho = f \left(\frac{y^2}{R_{20}} + \frac{z^2}{R_{02}} \right) \quad (22)$$

where f is an arbitrary positive function of one variable only. We note in passing that the foregoing arguments can easily be generalized to three dimensions for the class of systems with no parallel flow ($v_x=0$) if one reinter-

prets $\rho(y, z)$ as $\int \rho(x, y, z) dx$. The full density distribution corresponding to a quadratic velocity potential can then be expressed as an arbitrary positive function of two variables $\rho(x, y, z) = f(x, y^2/b^2 + z^2/c^2)$.

Let us now mention two famous examples of ellipsoidal equidensity surfaces. A popular example from classical hydrodynamics is the nonviscous, irrotational flow of a fluid with constant density inside an ellipsoidal container rotating uniformly around the x axis. The equidensity lines in the planes perpendicular to the rotation axis are conformal ellipses and hence a quadratic velocity potential follows. Therefore, the moment of inertia equals

$$\mathcal{J} = \frac{1}{5} \frac{(b^2 - c^2)^2}{b^2 + c^2} \quad (23)$$

where b and c are the half axes of the ellipsoid perpendicular to the cranking axis and $\mathcal{J}_{\text{rig}} = \frac{1}{5}$. This result has often been derived in the literature (see, e.g., [4]).

Another example concerns the cranked deformed harmonic-oscillator potential. This case is more extensively discussed in the context of nuclear physics (see Ref. [4]) where the actual rotations are, however, in between the extremes of irrotational and rigid flow and therefore do not concern us here any further. The ground-state wave function of a particle in a deformed-oscillator potential is a Gaussian and so is its density, $\rho = \exp[-(x^2/\alpha^2 + y^2/\beta^2 + z^2/\gamma^2)]$. The equidensity surfaces are again ellipsoids, the velocity potential is quadratic, and the quadrupole formula (23) for the moment of inertia applies (with $\beta = \sqrt{2/5}b$ and $\gamma = \sqrt{2/5}c$).

V. ROTATIONAL MAGNETIC MOMENT OF THE HYDROGEN MOLECULE

The hydrogen molecule is an instructive example of a cranked system where the quadrupole formula is not exact but yields a good first approximation. We shall consider it here with the aim of estimating the higher-order correction terms. We shall denote the internuclear distance by R , the position vectors of the protons by $\pm \mathbf{R}/2$, and the position vector of any electron by \mathbf{r} . We make two basic assumptions.

(i) Both protons are described as classical particles orbiting uniformly at a radius $R/2$ with a small angular velocity ω . Then the two electrons move quantum mechanically in the cranked potential² of the form $V(\mathbf{r}) = 1/|\mathbf{r} + \frac{1}{2}\mathbf{R}| + 1/|\mathbf{r} - \frac{1}{2}\mathbf{R}|$.

(ii) Irrotational flow is assumed as if both electrons were in the same single-particle state. This is in fact the dominant configuration. Due to correlations between electrons there is a small admixture of other configurations.

In the spirit of our method, as described in Sec. IV, we try to use as input the "best" density distribution but only a "trial" velocity field. First we present the calculation with a quadratic velocity potential field, and then we

²Throughout the present section we use atomic units.

explore the effect of further terms in the moment expansion up to the quartic velocity potential.

The physical situation is characterized by the fact that the electronic contribution to the mass current is small compared to the nuclear contribution because the electron has a small mass compared to the proton. On the other hand, the electronic contribution to the electric current is of the same order as the nuclear contribution. Therefore the magnetic moment due to rotational motion of the molecule has electronic and nuclear parts of the same magnitude. The rotational gyromagnetic factor g has a protonic term $g_p = 1$ and an electronic term given by the expression (see Appendix B)

$$g_e = -\frac{\mathcal{I}}{(R/2)^2}, \quad (24)$$

where \mathcal{I} is the moment of inertia of a single electron.

As a first approximation we use the quadrupole formula (18). If we take as input the experimental values [5] for $Q = 0.297$ and for $M = 1.825$ and the value of the equilibrium internuclear distance $R = 1.4$, we obtain the result

$$g_e^{(2)} = -0.099, \quad (25)$$

in fair agreement [5] with the experimental value $g_e^{\text{expt}} = -0.117$.

Next we consider the contribution of the quartic terms in the moment expansion. Since quartic moments of the density are not given experimentally, one has to rely on calculation. It is important that all needed moments are calculated consistently with the same density, since cancellations of large numbers may occur in solving the linear equations (13). As we wish only to estimate the contribution of the quartic velocity potential in order to check the convergence of the moment expansion, we use the density of a simple Heitler-London wave function,

$$\rho(\mathbf{r}) = \frac{\alpha^3}{\pi} \frac{e^{-\alpha|\mathbf{r} + \frac{1}{2}\mathbf{R}|} + e^{-\alpha|\mathbf{r} - \frac{1}{2}\mathbf{R}|}}{2(1+S)}, \quad (26)$$

where α is determined variationally and S is the overlap integral between atomic orbitals [6]. Using spheroidal coordinates one can calculate analytically all moments needed. Thanks to symmetry properties referred to earlier, the set of linear equations (13) reduces to three equations for the three unknown coefficients A_{11} , A_{31} , and A_{13} . For the values of the density parameters R and α we consider two options: (i) to optimize the ground-state energy, i.e., $R = 1.4$ and $\alpha = 1.17$ or (ii) to reproduce experimental values of Q and M , i.e., $R = 1.333$ and $\alpha = 1.173$. In both cases we calculated \mathcal{I} by means of (16) and we obtained as a correction with respect to the lowest order

$$g_e^{(4)} - g_e^{(2)} = \begin{cases} -0.0157 & \text{for (i)} \\ -0.0143 & \text{for (ii)}. \end{cases} \quad (27)$$

Finally we consider the fact that so far we only calculated the electronic gyromagnetic "function" $g_e(R)$ and that the experimental value is an average over the ground-state nuclear vibrational wave function $\chi_{v=0}(R)$. A numerical estimate, using for χ a harmonic-oscillator

ground state, yields a further correction to $g_e^{(4)}$,

$$\int \chi^2(R) g_e^{(4)}(R) dR - g_e^{(4)}(R = 1.4) = -0.001. \quad (28)$$

The addition of the above contributions would end up close to the experimental value. This agreement indicates that the contribution of higher-order moments ($N = 6$) and the effect of correlations, both electronic and nonadiabatic, are either small or cancel.

In order to assess the convenience of our method it may be useful to compare it with the work of Rychlewski [3], who presumably made the most complete study of the electromagnetic properties of H_2 . In his calculation, g_e is determined via the paramagnetic magnetizability by the so-called variation-perturbation method. There the electron correlation and the first-order perturbation by the external magnetic field are treated variationally. The basis functions for this expansion of both unperturbed and first-order perturbed wave functions are expressed in elliptic coordinates and contain nonlinear variational parameters. A number of 80 (65) terms, has been used for the unperturbed (the first-order) wave function.

Our method relies on the assumption that the probability flow of the H_2 ground state is irrotational. In the case of a two-electron wave function neglecting correlation, this assumption is exact. Therefore we expect our results to have the same quality as the self-consistent results mentioned by Rychlewski, which indeed is the case, i.e., a relative error of about 4% in each case.

It should be noted here also that Tilieu and Guy [7] have proposed a simple ansatz for the first-order perturbed ground state, which is in fact equivalent to our quadrupole formula. However, their idea, being completely *ad hoc*, does not contain the expansion in higher multiples and hence gives no clue as to the systematic improvement of the results.

VI. CONCLUSIONS

We have developed a method for the calculation of the moment of inertia for a quantum system which necessitates only the knowledge of a one-particle probability density of the ground state, in contradistinction to other methods which also require the excited states. The method is valid only for the case of irrotational probability flow. Nonirrotational effects may occur due to both Pauli and dynamical correlations. The corrections due to these effects are difficult to predict; their estimate would require at least the ground-state function rather than only its density.

Considering the important special case of irrotational flow, we have proposed a formula based on the expansion in moments of the ground-state probability density distribution. The first term in the series expansion yields the very simple relation stating that the moment of inertia equals the square of the quadrupole moment divided by the mean-square radius. The convergence of the series expansion of the moment of inertia is estimated on the example of the rotational gyromagnetic factor of the hydrogen molecule and is found to be good; the next higher term amounts to 10% of the leading term.

ACKNOWLEDGMENT

This work is supported by the IIKW-IISN, Belgium.

APPENDIX A

The probability density $\rho(\mathbf{R})$ and the probability current density $\mathbf{j}(\mathbf{R})$ associated with the wave function $\psi(\mathbf{r})$ are defined by

$$\rho(\mathbf{R}) = \langle \psi | \delta(\mathbf{r} - \mathbf{R}) | \psi \rangle, \quad (\text{A1})$$

$$\mathbf{j}(\mathbf{R}) = \frac{1}{2m} \langle \psi | \mathbf{p} \delta(\mathbf{r} - \mathbf{R}) + \delta(\mathbf{r} - \mathbf{R}) \mathbf{p} | \psi \rangle, \quad (\text{A2})$$

where $\delta(\mathbf{r} - \mathbf{R})$ is the Dirac delta distribution for the point \mathbf{R} . If we substitute \mathbf{j} in the definition of the dipole moment and integrate over \mathbf{R} first, we obtain the following relation:

$$\int \mathbf{R} \times \mathbf{j}(\mathbf{R}) d^3R = \int \psi(\mathbf{r}) (\mathbf{r} \times \mathbf{p}) \psi(\mathbf{r}) d^3r. \quad (\text{A3})$$

The angular-momentum \mathbf{L} of the mass flow and the magnetic-dipole moment $\boldsymbol{\mu}$ of the charge flow associated with ψ can then be expressed in terms of the current density or in terms of the velocity potential as

$$\mathbf{L}/m = \boldsymbol{\mu}(2c/e) = \int [\mathbf{R} \times \nabla \phi(\mathbf{R})] \rho(\mathbf{R}) d^3R. \quad (\text{A4})$$

The specific moment of inertia $\mathcal{J} = L_x/m\omega$ is then given by (10).

APPENDIX B

The definition of the electronic gyromagnetic factor g_e is given by expressing the electronic contribution to the

rotational magnetic moment of the hydrogen molecule in units of the nuclear magneton μ_N and relating it to the total molecular angular momentum J by the relation

$$\mu_e = \mu_N g_e J. \quad (\text{B1})$$

It may also be given in terms of the electronic orbital angular momentum l and expressed in Bohr magnetons,

$$\mu_e = -\mu_B l. \quad (\text{B2})$$

Hence,

$$g_e = -\frac{\mu_B}{\mu_N} \frac{l}{J}. \quad (\text{B3})$$

Using the relation between the moment of inertia and the angular momentum for a cranking velocity ω for both the protons and the electrons,

$$J = 2m_p \mathcal{J}_p \omega, \quad (\text{B4})$$

$$l = 2m_e \mathcal{J}_e \omega, \quad (\text{B5})$$

we obtain

$$\frac{l}{J} = \frac{\mathcal{J}_e}{\mathcal{J}_p} \frac{m_e}{m_p}. \quad (\text{B6})$$

Eliminating l/J from (B3) and (B4) we get

$$g_e = -\frac{\mathcal{J}_e}{\mathcal{J}_p}. \quad (\text{B7})$$

Now taking for the proton the classical moment of inertia $\mathcal{J}_p = (R/2)^2$, we arrive at the formula (24).

[1] D. R. Inglis, *Phys. Rev.* **96**, 1059 (1954).

[2] G. C. Wick, *Phys. Rev.* **73**, 51 (1948).

[3] J. Rychlewski, *Molecules in Physics, Chemistry, and Biology* (Kluwer, Dordrecht, New York, 1988), Vol. II, p. 207.

[4] A. Bohr and B. Mottelson, *Nuclear Structure* (Benjamin, New York, 1975), Vol. II, pp. 78 and 675.

[5] N. F. Ramsey, *Molecular Beams* (Oxford University Press, New York, 1958), Chap. 6.

[6] J. C. Slater, *Quantum Theory of Molecules and Solids* (McGraw-Hill, New York, 1963), p. 49.

[7] J. Tillieu and J. Guy, *C.R. Acad. Sci.* **239**, 1203 (1954).