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1962

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Abstract

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PHYSICS

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QUANTUM THEORY OF A ROTATING AND DEFORMABLE PARTICLE

(Presented by Academician V. A. Fock on VII 6, 1961)

The complexity of the many-body problem of quantum mechanics requires the construction of simplified models that would reflect certain essential properties of systems. For example, for an atomic nucleus and a complex molecule such properties are rotational and vibrational states. The quantum theory of a rotating and deformable particle proposed for describing these properties is constructed on the basis of the classical theory—of a body of homogeneous deformation as a mechanical system with nine degrees of freedom (with the center of mass fixed)—three rotational and six deformational. A closed theory of such a system, which is a generalization of the model of an absolutely rigid body, has been constructed by the author ⁽¹⁾ (see also the notation there).

§ 1. The equations of motion of the classical theory ⁽¹⁾ can be written in Hamiltonian form. Let us construct the Hamiltonian function H . As generalized coordinates we choose nine independent quantities χ_{ik} . The conjugate momenta are:

$$p_{ik} \equiv \partial T / \partial \dot{\chi}_{ik} = j_{ks}^0 \chi_{is}; \quad (1,1)$$

the inertial constants j_{ks}^0 are defined in ⁽¹⁾ (1,12). The Hamiltonian function

$$H \equiv \frac{\partial T}{\partial \dot{\chi}_{ik}} \dot{\chi}_{ik} - L = p_{ik} \dot{\chi}_{ik} - L = T + U + U^{\text{ex}}. \quad (1,2)$$

Denote the solution of system (1,1) with respect to $\dot{\chi}_{is}$ by:

$$\dot{\chi}_{ik} = I_{nm,ik}^0 p_{nm}; \quad (1,3)$$

$I_{nm,ik}^0$ is a square matrix of the ninth rank; its rows are numbered by the two first indices nm , and its columns by the two indices ik ; $I_{nm,ik}^0 = I_{ik,nm}^0$, i.e. this matrix is symmetric; it is inverse to the matrix

$$j_{jm,ik}^0 \equiv j_{mk}^0 \delta_{ni}. \quad (1,4)$$

Substituting (1,3) into (1,2), we obtain the Hamiltonian function explicitly:

$$H = \frac{1}{2} I_{nm,ik}^0 p_{nm} p_{ik} + U(\varepsilon_{ik}) + U^{\text{ex}}(\chi_{ik}), \quad (1,5)$$

where the deformational coordinates ε_{ik} are expressed through χ_{ni} :

$$\varepsilon_{ik} = \chi_{ni} \chi_{nk} - \delta_{ik}. \quad (1,6)$$

The angular momentum M_{ik} has the form

$$M_{ik} = \chi_{kn} p_{in} - \chi_{in} p_{kn}, \quad (1,7)$$

$$M_1 = \chi_{2n} p_{3n} - \chi_{3n} p_{2n}; \quad M_2 = \chi_{3n} p_{1n} - \chi_{1n} p_{3n}; \quad M_3 = \chi_{1n} p_{2n} - \chi_{2n} p_{1n}.$$

Let us compose the Poisson brackets for two functions F_1 and F_2 of the mechanical state, i.e. functions of the canonical variables χ_{nm} , p_{nm} . We retain the usual definition, namely

$$[F_1, F_2] \equiv \frac{\partial F_1}{\partial p_{nm}} \frac{\partial F_2}{\partial \chi_{nm}} - \frac{\partial F_1}{\partial \chi_{nm}} \frac{\partial F_2}{\partial p_{nm}}. \quad (1,8)$$

Hence, for the coordinates \varkappa_{rs} and momenta p_{rs} we obtain

$$[\varkappa_{rs}, \varkappa_{nm}] = 0; \quad [p_{rs}, p_{nm}] = 0; \quad [p_{rs}, \varkappa_{nm}] = \delta_{rs, nm}, \quad (1,9)$$

where the unit matrix of ninth rank $\delta_{rs, nm}$ is a generalization of the Kronecker symbol; it can be represented in the form of a product $\delta_{rs, nm} = \delta_{rn} \delta_{sm}$. The Poisson brackets for the components of the angular momentum of the amount of motion M_i have the form

$$[M_1, M_2] = -M_3; \quad [M_2, M_3] = -M_1; \quad [M_3, M_1] = -M_2. \quad (1,10)$$

Next we obtain that

$$[M^2, M_k] = 0 \quad (k = 1, 2, 3); \quad (1,11)$$

$$[M_1, \varkappa_{11}] = [M_1, \varkappa_{12}] = [M_1, \varkappa_{13}] = 0;$$

$$[M_1, \varkappa_{21}] = -\varkappa_{31}; \quad [M_1, \varkappa_{22}] = -\varkappa_{32}; \quad [M_1, \varkappa_{23}] = -\varkappa_{33}; \quad (1,12)$$

$$[M_1, \mathcal{U}_{31}] = \mathcal{U}_{21}; \quad [M_1, \mathcal{U}_{32}] = \mathcal{U}_{22}; \quad [M_1, \mathcal{U}_{33}] = \mathcal{U}_{23}.$$

The relations for M_2 and M_3 have an analogous form. The Poisson brackets $[M_1, p_{ik}]$ have the form (1,12) with \mathcal{U}_{ik} replaced by p_{ik} . If the external potential field is “central,” i.e., if

$$\mathcal{U}_{ks} \partial U^{\text{ex}} / \partial \mathcal{U}_{is} - \mathcal{U}_{is} \partial U^{\text{ex}} / \partial \mathcal{U}_{ks} = 0, \quad (1,13)$$

and also $Q_{ks} = 0$, then the Poisson brackets are

$$[H, M_k] = 0, \quad (1,14)$$

and hence it also follows that

$$[H, M^2] = 0. \quad (1,15)$$

If the external central field is stationary, then there is an energy integral $H = E_0$; in addition, from (1,14) we obtain three more first integrals of the motion,

$$M_k = M_k^0, \quad (1,16)$$

which, however, will not be independent because of the existence of (1,10). Two of the three M_i will be independent. As three independent first integrals of the motion one may choose H, M^2, M_3 .

§ 2. To construct the quantum theory of a rotating and deformable particle we shall follow the usual rules: assigning operators to dynamical quantities, we establish commutation relations between them by using the quantum analogue of Poisson brackets, namely

$$[F_1, F_2] \rightarrow \frac{i}{\hbar} (F_1 F_2 - F_2 F_1). \quad (2,1)$$

In what follows, without changing the notation of the dynamical quantities, we regard them as operators. From (1,9) we obtain

$$\mathcal{U}_{rs} \mathcal{U}_{nm} - \mathcal{U}_{nm} \mathcal{U}_{rs} = 0; \quad p_{rs} p_{nm} - p_{nm} p_{rs} = 0; \quad (2,2)$$

$$p_{rs} \mathcal{U}_{nm} - \mathcal{U}_{nm} p_{rs} = -i\hbar \delta_{rs, nm}. \quad (2,3)$$

From (1,10) we obtain

$$M_1 M_2 - M_2 M_1 = i\hbar M_3; \quad M_2 M_3 - M_3 M_2 = i\hbar M_1;$$

$$M_3 M_1 - M_1 M_3 = i\hbar M_2 \quad (2,4)$$

and from (1,11)

$$M^2 M_k - M_{kM}^2 = 0 \quad (k = 1, 2, 3). \quad (2,5)$$

From the commutation relations (2,4) and (2,5), as is known ⁽²⁾, there follows the spectrum of eigenvalues of M^2 and M_3 , namely

$$M^2 \psi = \hbar^2 j(j+1) \psi, \quad 2j \text{ is an integer}; \quad (2,6)$$

$$M_3 \psi = m\hbar \psi \quad (-j \leq m \leq +j).$$

Restricting ourselves to the case of a central external field, we obtain from (1.15)

$$HM^2 - M^2H = 0. \quad (2,7)$$

Thus, the eigenfunction of M^2 will also be an eigenfunction of the operators M_3 and H , i.e., a solution of the Schrödinger equation

$$H\psi = E\psi. \quad (2,8)$$

Let us write the explicit form of the Schrödinger equation in the representation in which the operators of the independent commuting variables χ_{rs} are simply operators of multiplication by χ_{rs} . For this it is necessary to construct the operators p_{nm} in the χ_{rs} representation. Then from (2.3), up to a unitary transformation, it follows that

$$p_{rs} = -i\hbar \partial / \partial \chi_{rs}. \quad (2,9)$$

To construct the operator H we turn to the Hamiltonian function (1.5) and see that, since $I_{nm,ik}^0$ are constants, by virtue of (2.2) substitution of the operators (2.9) gives an unambiguous expression for the operator H . Just as in the quantum mechanics of a point (a system of points), in order to obtain an unambiguous form of the operators one must use Cartesian coordinates, so in the theory developed here one must use the coordinates χ_{rs} . Thus, the Schrödinger equation (2.8) takes the form

$$H\psi = -\frac{1}{2}\hbar^2 I_{nm,ik}^0 \partial^2 \psi / \partial \chi_{nm} \partial \chi_{ik} + (U + U^{\text{ex}}) \psi = E\psi. \quad (2,10)$$

If the direction of the fixed axes $Ox_1x_2x_3$ is chosen so that they coincide with the principal axes of inertia of the body in the natural arrangement of the points, then $I_{ik}^0 = 0$ for $i \neq k$; $I_{11}^0 \equiv I_1^0$, $I_{22}^0 \equiv I_2^0$, $I_{33}^0 \equiv I_3^0$, and then the matrix $I_{nm,ik}^0$ assumes the simple form

$$I_{nm,ik}^0 = \frac{1}{I_k^0} \delta_{ni} \delta_{mk}; \quad (2,11)$$

here there is no summation over the index k , which we indicate by underlining.

§ 3. To investigate deformation, rotation, and the relation between them, we pass to other variables: six deformation coordinates ε_{nm} and three “orientational” coordinates ϑ_n , which we assume to be only independent of ε_{nm} and uniquely expressible in terms of χ_{rs} :

$$\vartheta_n = \vartheta_n(\chi_{11}, \chi_{12}, \chi_{13}, \chi_{21}, \chi_{22}, \chi_{23}, \chi_{31}, \chi_{32}, \chi_{33}) \quad (n = 1, 2, 3) \quad (3,1)$$

By ϑ_n one may, for example, understand φ_{ik} from ⁽¹⁾(1.3) or the Euler angles of a suitably rotating reference frame. From (1.6), (3.1), and (2.2) it follows for the corresponding operators that

$$\varepsilon_{nm} \varepsilon_{rs} - \varepsilon_{rs} \varepsilon_{nm} = 0; \quad \vartheta_n \vartheta_r - \vartheta_r \vartheta_n = 0. \quad (3,2)$$

The passage to the new variables can be carried out by applying the variational principle, as was already shown in Schrödinger’s first communication ⁽³⁾ (see also ⁽⁴⁾). However, it is simpler to perform a direct transformation to the new variables of the differential equation (2.10). Assuming that the nine coordinates χ_{ik} , by solving the system (1.6) and (3.1), are expressed in terms of the nine $\varepsilon_{nm}, \vartheta_n$ by single-valued continuous functions:

$$\chi_{ik} = \chi_{ik}(\varepsilon_{11}, \varepsilon_{22}, \varepsilon_{33}, \varepsilon_{12}, \varepsilon_{13}, \varepsilon_{23}, \vartheta_1, \vartheta_2, \vartheta_3) \quad (3,3)$$

and, consequently,

$$\psi(\chi_{ik}) = \psi(\varepsilon_{nm}, \vartheta_n), \quad (3,4)$$

we obtain

$$\partial / \partial \chi_{nm} = g_{nm,rs} \partial / \partial \varepsilon_{rs} + h_{nm,r} \partial / \partial \vartheta_r, \quad (3,5)$$

where $g_{nm,rs} \equiv \partial \varepsilon_{rs} / \partial \chi_{nm}$; $h_{nm,r} \equiv \partial \vartheta_r / \partial \chi_{nm}$. Substituting the operator (3.5) into equation (2.10), we obtain, restricting ourselves to the case (2.11), the Schrödinger equation in the coordinates $\varepsilon_{nm}, \vartheta_n$:

$$(T_1 + T_2 + T_3 + U + U^{\text{ex}})\psi = E\psi, \quad (3.6)$$

where

$$T_1 \equiv -\frac{\hbar^2}{2I_k^0} g_{nk,rs} \frac{\partial}{\partial \varepsilon_{rs}} \left(g_{nk,mp} \frac{\partial}{\partial \varepsilon_{mp}} \right); \quad T_2 \equiv -\frac{\hbar^2}{2I_k^0} h_{nk,r} \frac{\partial}{\partial \vartheta_r} \left(h_{nk,m} \frac{\partial}{\partial \vartheta_m} \right);$$

$$T_3 \equiv -\frac{\hbar^2}{2j_k^0} \left[g_{nk,rs} \frac{\partial}{\partial \varepsilon_{rs}} \left(h_{nk,m} \frac{\partial}{\partial \vartheta_m} \right) + h_{nk,r} \frac{\partial}{\partial \vartheta_r} \left(g_{nk,mp} \frac{\partial}{\partial \varepsilon_{mp}} \right) \right].$$

Further, using (1,6), we obtain:

$$g_{nk,rs} = \varkappa_{nr}, \quad k = s; \quad g_{nk,rs} = \varkappa_{ns}, \quad k = r; \quad g_{nk,rs} = 0, \quad k \neq s, \quad k \neq r. \quad (3.7)$$

The coefficients $h_{nk,m}$ are likewise uniquely expressed in terms of \varkappa_{nr} after choosing the explicit form of the functions (3,1). The \varkappa_{nr} in equation (3,6) must be replaced by the functions (3,3). Using only (3,7) and (1,6), the Schrödinger equation (3,6) can also be given the following form:

$$(H_{\text{df}} + H_{\text{rot}} + H_{\text{rd}})\psi = E\psi, \quad (3.8)$$

where

$$H_{\text{df}} \equiv -\frac{2\hbar^2}{j_s^0} \left[\varepsilon_{rm} \frac{\partial^2}{\partial \varepsilon_{rs} \partial \varepsilon_{ms}} + \frac{\partial^2}{\partial \varepsilon_{rs} \partial \varepsilon_{rs}} + \left(\varkappa_{nr} \frac{\partial \varkappa_{nm}}{\partial \varepsilon_{rs}} + \frac{1}{2} h_{ns,r} \frac{\partial \varkappa_{nm}}{\partial \vartheta_r} \right) \frac{\partial}{\partial \varepsilon_{ms}} \right] + U + U_{\text{df}}^{\text{ex}};$$

$$H_{\text{rot}} \equiv -\frac{\hbar^2}{2j_k^0} \left[h_{nk,r} \frac{\partial}{\partial \vartheta_r} \left(h_{nk,m} \frac{\partial}{\partial \vartheta_m} \right) + 2\varkappa_{nr} \frac{\partial h_{nk,m}}{\partial \varepsilon_{rk}} \frac{\partial}{\partial \vartheta_m} \right] + U_{\text{rot}}^{\text{ex}};$$

$$H_{\text{rd}} \equiv -\frac{2\hbar^2}{j_s^0} \varkappa_{nr} h_{ns,m} \frac{\partial^2}{\partial \varepsilon_{rs} \partial \vartheta_m}.$$

The interaction of rotation with deformation is very close and is described not only by the term H_{rd} ; in the term H_{df} the orientational coordinates ϑ_n are present, and in the term H_{rot} the coordinates ε_{nm} . Let us note that the names of the terms $H_{\text{df}}, H_{\text{rot}}, H_{\text{rd}}$, respectively as deformation energy, rotational energy, and the energy of the interaction of rotation with deformation, are somewhat

conventional and do not correspond to the separation of the energy in ⁽¹⁾ (2,13), because if the instantaneous rotation is defined by the vector Ω_i ⁽¹⁾ (2,3), which is quite natural, then the angles ϑ_n do not describe purely rotational degrees of freedom (i.e. the ϑ_n are not linear homogeneous functions of Ω_i).

The closed theory constructed is, in a certain sense, a generalization of the quantum theory of the asymmetric top investigated in works ⁽⁵⁻⁷⁾. For the phenomenological description of quantum systems it uses a small number of constants: the inertial constants j_k^0 and the elastic constants λ, μ , which enter into the expression for the internal potential energy

$$U = \tau \left(\frac{1}{2} \lambda \varepsilon^2 + \mu \varepsilon_{ik} \varepsilon_{ik} \right); \quad \varepsilon \equiv \varepsilon_{11} + \varepsilon_{22} + \varepsilon_{33}, \quad \tau = \tau_0 (1 + \varepsilon + \varepsilon_{ki} \varepsilon_{ki} + \Delta); \quad (3,9)$$

τ is the volume of the particle, and Δ is the determinant of ε_{ik} . We note that for a potential energy of the form (3,9) or ⁽¹⁾ (1,20), the total energy of the particle satisfies a fact known from nuclear physics—the independence, with respect to mass number, of the binding energy of the nucleus and of the density of its matter, calculated per nucleon.

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Received
28 VI 1961

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