Generalized coordinates in quantum mechanics

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A prescription is proposed for the construction of quantum-mechanical operators on the basis of the classical Lagrangian function in generalized coordinates. Integrals of the motion and particular dynamical systems are considered.

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CONTENTS

The transition from classical quantities to quantum operators is usually accomplished in rectilinear coordinates. But there are situations in which the kinetic energy in classical mechanics can be expressed only in terms of generalized coordinates and velocities. As an example, we cite the expression for the kinetic energy of the collective motions of the nucleons in an even-even axially symmetric nucleus[1]:

$$T=\frac{1}{2}g_{\mu\nu}\dot{q}^{\mu}\dot{q}^{\nu}=\frac{1}{2}\left(B\dot{\beta}^2+3\beta^2\dot{\theta}^2+3\beta^2\sin^2\theta\cdot\dot{\varphi}^2\right).$$

The space of configurations (β, θ, φ) in this example is not flat, since the curvature tensor is not equal to zero.

In the case in which the kinetic energy T is a homogeneous quadratic form in the velocities, there is every reason to suppose that in quantum mechanics the operator $\hat{T}$ is a Beltrami operator[2,3]; the situation is more complicated in the case of an arbitrary dynamical system. In this paper, we shall show how it is possible to construct the Hamiltonian and generalized-momentum operators by means of a regular process (see also Refs. 4–6). We shall also study the integrals of the motion of an arbitrary dynamical system on the basis of the classical Lagrangian function. As an illustration, we shall consider the following dynamical problems: a free gyroscope, the three-particle problem, and the problem of the rotation and small oscillations of a system of particles.

1. MOMENTUM AND HAMILTONIAN OPERATORS

We shall find the form of the Hamiltonian and generalized-momentum operators in configuration space for an arbitrary dynamical system. For this purpose, let us consider a classical dynamical system acted upon by both conservative and nonconservative forces (a magnetic field, Coriolis inertial forces, etc.). The Lagrangian function in this case has the form

$$L=\frac{1}{2}g_{\mu\nu}\dot{q}^{\mu}\dot{q}^{\nu}+a_{\mu}\dot{q}^{\mu}+T_0-V.$$

In the relative motion, T_0 represents the potential of the centrifugal inertial force. Calculating the Hamiltonian function, we obtain

$$H=\frac{1}{2}(p_{\mu}-a_{\mu})g^{\mu\nu}(p_{\nu}-a_{\nu})+V-T_0. \tag{1.1}$$

The configuration space Q, in which the coordinates of a representative point are the n generalized coordinates q^{μ} of the dynamical system, provides the most natural representation of this function. The metric of this space is specified by means of a linear element:

$$ds^2=g_{\mu\nu}dq^{\mu}dq^{\nu}\qquad (g_{\mu\nu}=g_{\nu\mu}).$$

We shall assume that the commutation relations for the generalized momenta and coordinates in the space Q are the same as in the Euclidean space for the rectilinear coordinates. It follows from this assumption that

$$\hat{p}_{(\mu)}=-i\frac{\partial}{\partial q^{\mu}}+\frac{\partial E}{\partial q^{\mu}}=e^{-iF}\left(-i\frac{\partial}{\partial q^{\mu}}\right)e^{iF}\qquad (\hbar=1).$$

Putting $F=f-i\ln c$, we have

$$\hat{p}_{(\mu)}=e^{-if}c^{-1}\left(-i\frac{\partial}{\partial q^{\mu}}\right)ce^{if}.$$

By means of a unitary transformation, we can eliminate the arbitrary function f. Then

$$\hat{p}_{(\mu)}=c^{-1}\left(-i\frac{\partial}{\partial q^{\mu}}\right)c. \tag{1.2}$$

In quantum mechanics, we shall seek the operator $\hat{H}$ corresponding to the classical function H in (1.1) in the form

$$\hat{H}=\frac{1}{2}A(q)(\hat{p}_{(\mu)}+a_{\mu})g^{\mu\nu}B(q)(\hat{p}_{(\nu)}a_{\nu})D(q)+V-T_0. \tag{1.3}$$

It follows from the condition that $\hat{H}$ is Hermitian that $D=A$. Using (1.2), we obtain

$$\hat{H}=\frac{1}{2}AC^{-1}\frac{\partial}{\partial q^{\mu}}g^{\mu\nu}B\frac{\partial}{\partial q^{\nu}}AC+iA^2Ba^{\mu}\frac{\partial}{\partial q^{\mu}}+\frac{i}{2}AC^{-1}\frac{\partial}{\partial q^{\mu}}(ABCa^{\mu})+\frac{i}{2}ABC^{-1}a^{\nu}\frac{\partial}{\partial q^{\nu}}(AC)+\frac{1}{2}A^2Ba^{\mu}a_{\mu}. \tag{1.4}$$

From the requirement of invariance of the last three terms in (1.4), we find

$$A^2B=\text{const}=1,\quad ABC^{-1}=\text{const},\quad CA^{-1}=k\sqrt{g}$$

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(k is a constant). It follows from the correspondence principle that const=1 in the first case. Substituting the resulting values of A, B, and C into (1.4) and (1.2), we finally obtain

$$\hat{H} = -\frac{1}{2\sqrt{g}}\frac{\partial}{\partial q^{\mu}} g^{\mu\nu}\sqrt{g}\,\mu\frac{\partial}{\partial q^{\nu}} + ia^{\mu}\frac{\partial}{\partial q^{\mu}} + \frac{i}{2\sqrt{g}}\frac{\partial}{\partial q^{\mu}}(\sqrt{g}a^{\mu}) + \frac{1}{2}a^{\mu}a_{\mu} + V - T_0,$$

$$\hat{p}_{(\mu)} = g^{-1/4}\left(-i\frac{\partial}{\partial q^{\mu}}\right)g^{1/4}. \qquad (1.5)$$

Thus, the requirement of invariance of only three terms in (1.4) implies invariance of the Hamiltonian operator $\hat{H}$. In view of the fact that $\hat{p}_{(\mu)}$ are not components of a vector, we enclose the index μ in parentheses. Since $g_{\mu\nu}\dot{q}^{\mu}\dot{q}^{\nu}$ is a positive-definite form, the eigenvalues of the operator $\hat{H}$ in (1.5) with $V=0$ and $T_0=0$ are non-negative. Depending on the topology of the space, the spectrum of eigenvalues will be either continuous or discrete. With a Euclidean topology and $a_{\mu} \to 0$ at infinity, the spectrum is continuous. If the discussion is mathematically rigorous, this is the case for the motion of a particle in a real magnetic field.

2. INTEGRALS OF THE MOTION LINEAR IN THE MOMENTA

For our purposes, we are interested in only integrals of the motion that can be represented in covariant form. In the case of complete separation of the variables, the separation constants are also integrals of the motion. If there are no cyclic coordinates, all these integrals are quadratic functions of the momenta; however, since the variables are separated in certain curvilinear coordinate systems, these integrals cannot be represented in covariant form. Let us consider integrals linear in the momenta.

If the following conditions are satisfied,

$$D^{\mu;\nu} + D^{\nu;\mu} = D_{\nu;\mu} + D_{\mu;\nu} = 0, \qquad (2.1)$$

$$D^{\mu}_{;\nu}a^{\nu} - a^{\mu}_{;\nu}D^{\nu} - g^{\mu\nu}\frac{\partial N_0}{\partial q^{\nu}} = 0, \qquad (2.2)$$

$$D^{\mu}\frac{\partial}{\partial q^{\mu}}\left(V - T_0 + \frac{1}{2}a^{\nu}a_{\nu}\right) + a^{\mu}\frac{\partial N_0}{\partial q^{\mu}} = 0 \qquad (2.3)$$

the quantity $N = D^{\mu}p_{\mu} + N_0$ is an integral of the motion of the classical system (1.1).

It follows from the condition (2.1) that $D_{\mu}(q)$ forms a Killing vector of the metric $g_{\mu\nu}(q)$. The number m of independent Killing vectors and the dimensionality n of the space Q are related by

$$m \leqslant \frac{1}{2}n(n+1).$$

The equality holds in the case of a space of constant curvature.[7] It follows from the equation $D^{\mu;\nu} + D^{\nu;\mu}$ that

$$D^{\mu}_{;\mu} = 0, \qquad (2.4)$$

i.e., the covariant divergence of a contravariant Killing vector is equal to zero.

In quantum mechanics, the tensor operator

$$\hat{N} = \frac{1}{2}(D^{\mu}\hat{p}_{(\mu)} + \hat{p}_{(\mu)}D^{\mu}) + N_0 \qquad (2.5)$$

is also an integral of the motion if, in addition to Eqs. (2.1), (2.2), and (2.3), the following two conditions are also satisfied:

$$\frac{1}{\sqrt{g}}\frac{\partial}{\partial q^{\nu}}\{\sqrt{g}(D^{\mu;\nu} + D^{\nu;\mu})\} = g^{\mu\nu}\frac{\partial}{\partial q^{\nu}}(D^{\rho}_{;\rho}), \qquad (2.6)$$

$$\frac{1}{\sqrt{g}}\frac{\partial}{\partial q^{\nu}}\left[\sqrt{g}\left(D^{\nu}_{;\mu}a^{\mu} - a^{\nu}_{;\mu}D^{\mu} - g^{\nu\mu}\frac{\partial N_0}{\partial q^{\mu}}\right)\right] = a^{\nu}\frac{\partial}{\partial q^{\nu}}(D^{\rho}_{;\rho}). \qquad (2.7)$$

It is easy to see that when (2.4) is taken into account the conditions (2.6) and (2.7) are satisfied automatically.

Making use of (2.4), we obtain for $\hat{N}$ an expression of the form

$$\hat{N} = -iD^{\mu}\frac{\partial}{\partial q^{\mu}} + N_0. \qquad (2.8)$$

Thus, if N is an integral of the motion in classical mechanics, the operator $\hat{N}$ in (2.8) corresponding to N in quantum mechanics is also an integral of the motion. We note that the maximum number of integrals in quantum mechanics occurs in the case of "inertial" motion in a space of constant curvature, and this number is $\frac{1}{2}n(n+1)$, where n is the dimensionality of the space. If the classical Poisson bracket is

$$\{NM\} = K, \qquad (2.9)$$

where $N = D^{\mu}p_{\mu} + N_0$, $M = E^{\mu}p_{\mu} + M_0$, $K = F^{k}p_{k} + K_0$ and $D^{\mu}_{;\mu} = 0$, $E^{\mu}_{;\mu} = 0$

$$F^{\mu}_{;\mu} = 0 \text{ and } [\hat{N}\hat{M}] = -i\hat{K}. \qquad (2.10)$$

Let us consider a simple example. The kinetic energy of a solid body with moments of inertia $I_1 = I_2 = I_3 = I$, expressed in terms of the Euler angles and their derivatives, has the form

$$T = \frac{I}{2}(\dot{\theta}^2 + \dot{\psi}^2 + \dot{\varphi}^2 + 2\dot{\psi}\dot{\varphi}\cos\theta). \qquad (2.11)$$

The space Q in (2.11) is not flat. The Ricci tensor and the Riemann–Christoffel tensor in this case can be represented in the form

$$R_{\mu\nu} = -(N-1)Kg_{\mu\nu}, \quad R_{\mu\nu\rho\sigma} = K(g_{\rho\nu}g_{\mu\sigma} - g_{\sigma\nu}g_{\mu\rho}),$$

where $N = 3$ and $K = -\frac{1}{4}$.

Consequently, the space Q is a space of constant curvature. Let us find the integrals of the motion which represent the projections of the angular momentum onto the moving and fixed axes.

It follows from (2.11) that

$$\dot{\theta} = I^{-1}p_{\theta}, \quad \dot{\psi} = (I\sin^2\theta)^{-1}\cdot(p_{\psi} - p_{\varphi}\cos\theta),$$

$$\dot{\varphi} = (I\sin^2\theta)^{-1}\cdot(p_{\varphi} - p_{\psi}\cos\theta).$$

The angular-momentum projections $J_{(1)}$, $J_{(2)}$, and $J_{(3)}$ onto the moving axes are $J_{(1)} = I\omega_1$, $J_{(2)} = I\omega_2$, and $J_{(3)} = I\omega_3$, or

$$\left.\begin{aligned} J_{(1)} &= D^{\mu}_{(1)}p_{\mu} = \cos\varphi\cdot p_{\theta} + \frac{\sin\varphi}{\sin\theta}p_{\psi} - \operatorname{ctg}\theta\cdot\sin\varphi\cdot p_{\varphi},\\ J_{(2)} &= D^{\mu}_{(2)}p_{\mu} = -\sin\varphi\cdot p_{\theta} + \frac{\cos\varphi}{\sin\theta}p_{\psi} - \operatorname{ctg}\theta\cos\varphi\cdot p_{\varphi},\\ J_{(3)} &= D^{\mu}_{(3)}p_{\mu} = p_{\varphi}. \end{aligned}\right\} \qquad (2.12)$$

On the basis of (2.8), we have the following expressions for the operators of the angular-momentum projections in the moving coordinate system:

$$\left.\begin{aligned} \hat{J}_{(1)} &= -i\left(\cos\varphi\frac{\partial}{\partial\theta} + \frac{\sin\varphi}{\sin\theta}\frac{\partial}{\partial\psi} - \operatorname{ctg}\theta\cdot\sin\varphi\cdot\frac{\partial}{\partial\varphi}\right),\\ \hat{J}_{(2)} &= -i\left(-\sin\varphi\frac{\partial}{\partial\theta} + \frac{\cos\varphi}{\sin\theta}\frac{\partial}{\partial\psi} - \operatorname{ctg}\theta\cdot\cos\varphi\cdot\frac{\partial}{\partial\varphi}\right),\\ \hat{J}_{(3)} &= -i\frac{\partial}{\partial\varphi}. \end{aligned}\right\} \qquad (2.13)$$

Similarly, by considering the projections of ω onto the fixed axes, we obtain

$$J_{(x)}=D^{\mu}_{(x)}p_\mu=\cos\psi\cdot p_\theta-\operatorname{ctg}\theta\cdot\sin\psi\cdot p_\psi+\frac{\sin\psi}{\sin\theta}p_\varphi,$$

$$J_{(y)}=D^{\mu}_{(y)}p_\mu=\sin\psi\cdot p_\theta+\operatorname{ctg}\theta\cdot\cos\psi\cdot p_\psi-\frac{\cos\psi}{\sin\theta}p_\varphi,$$
$$J_{(z)}=D^{\mu}_{(z)}p_\mu=p_\psi.$$

In quantum mechanics,

$$\hat{J}_x=-i\left(\cos\psi\frac{\partial}{\partial\theta}-\operatorname{ctg}\theta\cdot\sin\psi\frac{\partial}{\partial\psi}+\frac{\sin\psi}{\sin\theta}\frac{\partial}{\partial\varphi}\right),$$

etc.

The commutation relations are readily obtained by making use of (2.9). The maximally symmetric three-dimensional space in (2.11) has six independent Killing vectors: $D^{\mu}_{(1)}$, $D^{\mu}_{(2)}$, $D^{\mu}_{(3)}$, $D^{\mu}_{(x)}$, $D^{\mu}_{(y)}$, and $D^{\mu}_{(z)}$. We note that although (2.11) describes free motion, the operator $\hat{T}$ has a discrete spectrum. This is due to the topological characteristics of the space of rotations.[8]

In conclusion, we consider two particular dynamical problems.

3. THREE PARTICLES

To describe the motion of three particles, we introduce the Jacobi coordinates

$$\mathbf{R}=\mathbf{r}_2-\mathbf{r}_1,\quad \mathbf{r}=\mathbf{r}_3-\frac{m_1\mathbf{r}_1+m_2\mathbf{r}_2}{m_1+m_2},\qquad \mathbf{R}_c=\frac{m_1\mathbf{r}_1+m_2\mathbf{r}_2+m_3\mathbf{r}_3}{m_1+m_2+m_3}.$$

The kinetic energy of the system is

$$T=\frac{1}{2}\left[\frac{m_1m_2}{m_1+m_2}\dot{\mathbf{R}}^2+\frac{m_3(m_1+m_2)}{m_1+m_2+m_3}\dot{\mathbf{r}}^2+(m_1+m_2+m_3)\dot{\mathbf{R}}_c^2\right].$$

We place the origin of the coordinate system at the center of mass ($\mathbf{R}_c=0$) and put

$$\frac{m_3(m_1+m_2)}{m_1+m_2+m_3}=1,\qquad \frac{m_1m_2}{m_1+m_2}=\mu;$$

then

$$T=\frac{1}{2}\mu\dot{\mathbf{R}}^2+\frac{1}{2}\dot{\mathbf{r}}^2. \tag{3.1}$$

Thus, having eliminated the coordinates of the center of mass, we have reduced the problem to the problem of the motion of two quasiparticles with masses μ and 1.

With the choice of the variables R, θ, φ, x, y, and z (in the fixed space Σ), the potential energy depends on the angles; to avoid this, we introduce a moving coordinate system Σ'. The z axis of the system Σ' is directed along the vector $\mathbf{R}$. The position of $\mathbf{R}$ in Σ is characterized by the angles θ and φ. We shall assume that Σ' is obtained from Σ by successive rotations through the Euler angles $(\varphi+\frac{1}{2}\pi,\ \theta,0)$. In the problem of the motion of a particle in the field of two centers, we use an elliptic coordinate system whose origin bisects the line joining the centers. Consequently, we make the substitution

$$\mathbf{r}\to\mathbf{r}+aR\mathbf{k}\qquad\left(a=\frac{m_1-m_2}{2(m_1+m_2)}\right).$$

The components of the angular velocity $\boldsymbol{\omega}$ in Σ' are $(\dot\theta,\dot\varphi\sin\theta,\ \dot\varphi\cos\theta)$. We represent the absolute velocity $\dot{\mathbf{r}}$ in (3.1) as the sum of the relative and transport velocities:

$$\dot{\mathbf{r}}\to\mathring{\mathbf{r}}+[\boldsymbol{\omega}(\mathbf{r}+aR\mathbf{k})]+a\dot{R}\mathbf{k}$$

(here $\mathring{\mathbf{r}}$ denotes the velocity in Σ', and $\mathbf{i}$, $\mathbf{j}$, and $\mathbf{k}$ are the unit vectors of the moving coordinate system). With this substitution, the Lagrangian function is

$$L=\frac{1}{2}\mu\dot{\mathbf{R}}^2+\frac{1}{2}(\mathring{\mathbf{r}}+[\boldsymbol{\omega}(\mathbf{r}+aR\mathbf{k})]+a\dot{R}\mathbf{k})^2-V(R,\ x,\ y,\ z). \tag{3.2}$$

Calculating the Hamiltonian function, we obtain

$$\begin{aligned}H=&\frac{1}{2\mu}\Big[(P_R-ap_z)^2+R^{-2}(p_\theta-l_x+aRp_y)^2\\&+R^{-2}\sin^{-2}\theta\,(p_\varphi-l_y\sin\theta-l_z\cos\theta-aRp_x\sin\theta)^2\Big]\\&+\frac{1}{2}\mathbf{p}^2+V(R,\ x,\ y,\ z)\end{aligned} \tag{3.3}$$

(p_x, p_y, p_z; l_x, l_y, l_z are the projections onto the moving axes of the momentum and the angular of the second quasiparticle). The fundamental determinant is

$$g=R^4\sin^2\theta.$$

The Hamiltonian function (3.3) in quantum mechanics corresponds to the following operator $\hat{H}(\hbar=1)$:

$$\begin{aligned}\hat{H}=&-\frac{1}{2\mu}\Big[\left(\frac{\partial}{\partial R}-iaR\hat{p}_z\right)^2+2R^{-1}\left(\frac{\partial}{\partial R}-iaR\hat{p}_z\right)\\&+R^{-2}\left(\frac{\partial}{\partial\theta}-i\hat{l}_x+iaR\hat{p}_y\right)^2+R^{-2}\operatorname{ctg}\theta\cdot\left(\frac{\partial}{\partial\theta}-i\hat{l}_x+iaR\hat{p}_y\right)\\&+R^{-2}\sin^{-2}\theta\left(\frac{\partial}{\partial\varphi}-i\hat{l}_z\cos\theta-i\hat{l}_y\sin\theta-iaR\sin\theta\cdot\hat{p}_x\right)^2\Big]\\&+\frac{1}{2}\hat{\mathbf{p}}^2+V(R,\ x,\ y,\ z).\end{aligned} \tag{3.4}$$

Another method of constructing the operator $\hat{H}$ is given in Ref. 9.

The total angular momentum of the system is equal to the sum of the angular momenta of the two quasiparticles. The angular-momentum projections of the first of them onto the moving axes are $(\mu R^2\dot\theta,\ \mu R^2\sin\theta\cdot\dot\varphi,0)$, and those of the second are $(l_x=aRp_y,\ l_y+aRp_x,\ l_z)$. The quantities l_x, l_y, and l_z are the projections of the angular momentum with respect to a point displaced from the origin along the z axis by a distance aR.

Since

$$p_\theta=\mu R^2\dot\theta+l_x-aRp_y,$$
$$p_\varphi=\mu R^2\sin^2\theta\cdot\dot\varphi+l_y\sin\theta+l_z\cos\theta+aRp_x\sin\theta,$$

the square of the total angular momentum is

$$\mathbf{K}^2=p_\theta^2+\sin^{-2}\theta\,(p_\varphi-l_z\cos\theta)^2+l_z^2. \tag{3.5}$$

The projections of the total angular momentum in Σ' are

$$\left.\begin{aligned}K_x&=-\sin\varphi\cdot p_\theta-\operatorname{ctg}\theta\cdot\cos\varphi\cdot(p_\varphi-l_z\cos\theta)+\sin\theta\cdot\cos\varphi\cdot l_z,\\K_y&=\cos\varphi\cdot p_\theta-\operatorname{ctg}\theta\cdot\sin\varphi\cdot(p_\varphi-l_z\cos\theta)+\sin\theta\cdot\sin\varphi\cdot l_z,\\K_z&=p_\varphi.\end{aligned}\right\} \tag{3.6}$$

The functions D^{μ} in (3.6) satisfy the condition (2.4). Consequently, in quantum mechanics ($\hbar=1$)

$$\left.\begin{aligned}\hat{K}_x&=i\sin\varphi\frac{\partial}{\partial\theta}+i\operatorname{ctg}\theta\cdot\cos\varphi\cdot\frac{\partial}{\partial\varphi}+\frac{\cos\varphi}{\sin\theta}\hat{l}_z,\\\hat{K}_y&=-i\cos\varphi\frac{\partial}{\partial\theta}+i\operatorname{ctg}\theta\cdot\sin\varphi\cdot\frac{\partial}{\partial\varphi}+\frac{\sin\varphi}{\sin\theta}\hat{l}_z,\\\hat{K}_z&=-i\frac{\partial}{\partial\varphi}\end{aligned}\right\} \tag{3.7}$$

(here $\hat{l}_z$ is the projection in Σ', and $\hat{K}_x$, $\hat{K}_y$, and $\hat{K}_z$ are in Σ'). Replacing the physical quantities in (3.5) by operators, we obtain

$$\hat{\mathbf{K}}^2=-\left[\sin^{-1}\theta\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)+\sin^{-2}\theta\left(\frac{\partial}{\partial\varphi}-i\hat{l}_z\cos\theta\right)^2\right]+\hat{l}_z^2. \tag{3.8}$$

In the case of a diatomic molecule, we can assume that the center of mass coincides with the center of mass of the nuclei. In this case, by putting $a=0$, replacing the angular momentum of the second quasiparticle in (3.4), (3.7), and (3.8) by the sum of the angular momenta of all the electrons, and replacing $\hat{\mathbf{p}}^2$ by $\sum_i \hat{\mathbf{p}}_i^2$, we obtain the operators $\hat{H}$, $\hat{K}_x$, $\hat{K}_y$, $\hat{K}_z$, and $\hat{\mathbf{K}}^2$ for the diatomic molecule.

4. ROTATION AND SMALL OSCILLATIONS OF A SYSTEM OF PARTICLES

In quantum mechanics, we do not have the right to impose either finite or differential constraints on a system. Let us consider a system of particles characterized by moments of inertia in an "equilibrium" position is and suppose that the deviation from the "equilibrium" position is small. The mass of any particle can be taken to be equal to unity in the corresponding coordinate transformation. The kinetic energy T of the system is

$$T=\frac{1}{2}\sum_i{}'(\dot{\mathbf{u}}_i+[\boldsymbol{\omega}\mathbf{r}_{0i}]+[\boldsymbol{\omega}\mathbf{u}_i])^2;$$

here $\mathbf{r}_{0i}$ and $\mathbf{u}_i$ are vectors characterizing the "equilibrium" position and the deviation from this position of particle i in the system Σ'. The system Σ' rotates with angular velocity $\boldsymbol{\omega}$ with respect to the fixed system Σ. Neglecting $\omega^2 u_i^2$ and $\omega^2 u_i r_{0i}$ and using the fact that[10]

$$\frac{d}{dt}\sum_i[\mathbf{r}_{0i}\mathbf{u}_i]=0;$$

we obtain

$$T=\frac{1}{2}\sum_i(\dot{\mathbf{u}}_i+2\boldsymbol{\omega}[\mathbf{u}_i\dot{\mathbf{u}}_i])^2+T_0.$$

Here T_0 is the kinetic energy of a gyroscope. We introduce the normal coordinates

$$\mathbf{u}_i=\sum_\alpha \mathbf{a}_{i\alpha}q_\alpha.$$

In this case,

$$T=\frac{1}{2}\sum_\alpha \dot{q}_\alpha^2+\boldsymbol{\omega}\sum_\alpha\sum_\beta \mathbf{b}_{\alpha\beta}q_\alpha\dot{q}_\beta+T_0.$$

where $\mathbf{b}_{\alpha\beta}=\sum_i[\mathbf{a}_{i\alpha}\mathbf{a}_{i\beta}]=-\mathbf{b}_{\beta\alpha}$ and $\sum_i\mathbf{a}_{i\alpha}\mathbf{a}_{i\beta}=\sigma_{\alpha\beta}$. We call attention to the fact that $|\mathbf{b}_{\alpha\beta}|\leq 1$. If for fixed α and β we have

$$\mathbf{a}_{i\alpha}\perp\mathbf{a}_{i\beta},\quad |\mathbf{a}_{i\alpha}|=|\mathbf{a}_{i\beta}|,\quad [\mathbf{a}_{i\alpha}\mathbf{a}_{i\beta}]=a_{i\alpha}^2\mathbf{n}$$

and if the unit vector $\mathbf{n}$ is independent of i, then in this case (and only in this case) $|\mathbf{b}_{\alpha\beta}|=1$.

In the case of a symmetric gyroscope,

$$T=\frac{1}{2}\sum_\alpha \dot{q}_\alpha^2+\boldsymbol{\omega}\sum_\alpha\sum_\beta \mathbf{b}_{\alpha\beta}q_\alpha\dot{q}_\beta+\frac{1}{2}I_1(\dot{\psi}^2\sin^2\theta+\dot{\theta}^2)+\frac{1}{2}I_3(\dot{\psi}\cos\theta+\dot{\varphi})^2. \tag{4.1}$$

It follows from (4.1) that

$$p_\varphi=I_3(\dot{\psi}\cos\theta+\dot{\varphi})+l_z,$$
$$p_\theta=I_1\dot{\theta}+l_x\cos\varphi-l_y\sin\varphi,$$
$$p_\psi=I_1\dot{\psi}\sin^2\theta+I_3(\dot{\psi}\cos\theta+\dot{\varphi})\cos\theta+l_x\sin\theta\cdot\sin\varphi+l_y\sin\theta\cos\varphi+l_z\cos\theta;$$

here l_x, l_y, and l_z are the projections of the "oscillating angular momentum" onto the moving axes:

$$l_x=\sum_\alpha\sum_\beta b_{\alpha\beta}^{(x)}q_\alpha p_\beta\ ,\ \text{etc},$$

(we have neglected terms of the form $\omega^2 q_\alpha q_\beta$).

Replacing the velocities by the momenta in (4.1), we obtain

$$T=\frac{1}{2}\sum p_\alpha^2+\frac{1}{2I_1}[(\mathbf{J}^2-J_z^2)+l_x^2+l_y^2-2(J_xl_x+J_yl_y)]+\frac{1}{2I_3}(J_z-l_z)^2.$$

In quantum mechanics, the physical quantities must be replaced by the corresponding operators.

Since $|\mathbf{b}_{\alpha\beta}|\leq 1$, the eigenvalue $\hat{l}_z$ is not in general equal to an integer. In the case of a linear molecule, $\mathbf{b}_{\alpha\beta}=\mathbf{n}$ (where $\mathbf{n}$ is a unit vector directed along the axis of the molecule), $\hat{l}_\alpha^{(z)}=x_\alpha p_{y\alpha}-y_\alpha p_{x\alpha}$, and the eigenvalues $\hat{l}_\alpha^{(z)}$ are integers.

Thus, we have constructed the Hamiltonian operators and the operators of the generalized momenta on the basis of the Lagrangian function in generalized coordinates. We have proved that the operators linear in the momenta which correspond to integrals of the motion in classical mechanics are also integrals of the motion in quantum mechanics.

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