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THE GENERALIZED SYMMETRICAL JACOBIS' COORDINATES FOR THE NON-RELATIVISTIC MANY-BODY PROBLEM

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Обобщенные симметричные координаты Якоби для нерелятивистской задачи многих тел

В работе введены обобщенные симметричные координаты Якоби для нерелятивистской системы многих тел с различными массами. Эти координаты позволяют исключить центр инерции системы тел таким образом образом, что оставшаяся часть классического или квантовомеханического гамильтониана симметрична относительно перестановок всех тел.

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Lukáč I.

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The Generalized Symmetrical Jacobis' Coordinates for the Non-Relativistic Many-Body Problem

The generalized symmetrical Jacobis' coordinates for the non-relativistic many-body problem are introduced. These coordinates permit the elimination of the centre-of-mass of the system in such a way that the remaining part of the Hamiltonian (classical or quantum-mechanical) is symmetrical in regards to the permutation of all particles.

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Introduction

The classical and quantum-mechanical many-particle problem is a problem which has been very attractive for a great number of investigators for many years. In spite of the principle difference of the classical and the quantum-mechanical non-relativistic many-particle problem there is a general feature in the solution of these two problems. Such a common feature of the mentioned problems is the elimination of three degrees of freedom connected with the motion of centre-of-mass of the many-particle system and the introduction of some new independent coordinates. Let's suppose that the many-particle system contains an N number of different mass particles which we shall denote as m_1, m_2 ... m_N, where $m_1 \geqslant m_2 \geqslant \ldots \geqslant m_N$. The system of N particles has 3N degrees of freedom. The main task of the classical or quantum mechanics of the N free or interacting particles consists in the elimination of centre-of-mass of the system.

It is well known that the problem of the elimination of the centre-of-mass for the three-particle system was solved for the first time by C.G.J. Jacobi in his memoire/1/ in 1843. At the present time these (relative) coordinates are called the Jacobis' ones for the three-body problem. These coordinates were generalized by M. Allegret in his work/2/ for the case of N bodies in 1875.

The classical system of the N free particles is characterized by two quantities: the kinetic energy T_0 and the moment $\vec{M}_0$ in the following form

$$T_0 = \frac{1}{2} \sum_{i=1}^{N} m_i \dot{\vec{R}}_i^2 , \quad \vec{M}_0 = \sum_{i=1}^{N} m_i \, [\vec{R}_i \times \dot{\vec{R}}_i] , \qquad (1)$$

where the point over vectors $\dot{\vec{R}}_i$ indicates the time derivation. The Jacobis' coordinates for the N-particle system having the obvious geometrical meaning are introduced as following[3,4]:

$$\vec{r}_o = m_o^{-1} \sum_{i=1}^{N} m_i \vec{R}_i \ , \quad m_o = \sum_{i=1}^{N} m_i \ ,$$

$$\vec{r}_\alpha = \vec{R}_{\alpha+1} - \left(\sum_{\beta=1}^{\alpha} m_\beta \vec{R}_\beta \right) \left(\sum_{\beta=1}^{\alpha} m_\beta \right)^{-1} , \qquad (2)$$

$$\alpha = 1,2, \ldots N-1 ,$$

where $\vec{r}_o$ is radius-vector of the centre-of-mass of the system, the coordinate $\vec{r}_\alpha$ represents the vector connecting the centre-of-mass of the sub-system of particles with the numbers 1,2, ... α and the particle with the number $\alpha + 1$. The inverse transformation to the one expressed by (2) is:

$$\vec{R}_i = \vec{r}_o - \sum_{k=1}^{N} \left[m_{k+1} \vec{r}_k \left(\sum_{j=1}^{k} m_j \right)^{-1} \right] +$$

$$+ \left(\sum_{k=1}^{i-1} m_k \right) \left(\sum_{j=1}^{i} m_j \right)^{-1} \vec{r}_{i-1} \ .$$

The classical energy E_o of N particles interacting by means of the potential $V(\vec{R}_1, \vec{R}_2, \ldots \vec{R}_N)$ may be expressed by means of the Jacobis' coordinates (2) as:

$$E_o = \frac{1}{2} \sum_{i=1}^{N} m_i \dot{\vec{R}}_i^2 + V(\vec{R}_1, \vec{R}_2, \ldots \vec{R}_N) =$$

$$= \frac{1}{2} m_o \dot{\vec{r}}_o^2 + \frac{1}{2} \sum_{\alpha=1}^{N-1} \mu_\alpha r_\alpha^2 + V(\vec{r}_1, \vec{r}_2, \ldots \vec{r}_{N-1}). \qquad (3)$$

The quantities μ_α in the formula of the kinetic energy (3) have - in the present case - the following simple form:

$$\mu_\alpha^{-1} = m_{\alpha+1}^{-1} + \left(\sum_{\beta=1}^{\alpha} m_\beta\right)^{-1}, \text{ i.e. } \mu_\alpha = m_{\alpha+1}\left(\sum_{\beta=1}^{\alpha} m_\beta\right)\left(\sum_{\beta=1}^{\alpha+1} m_\beta\right)^{-1}.$$

The principal defect of the Jacobis' coordinates entered in the form (2) is connected with this fact that they are not symmetrical in regards to the permutation of all particles. It is a very serious defect because,e.g.,the quantum-mechanical solutions $\psi_{[E]}$ $(\vec{R}_1, \vec{R}_2, \ldots \vec{R}_N)$ of Schrödinger's equation for N-particle problem

$$\left[-\frac{\hbar^2}{2}\sum_{i=1}^{N} m_i^{-1}\frac{\partial^2}{\partial \vec{R}_i^2} + V(\vec{R}_1, \vec{R}_2, \ldots \vec{R}_N) - E\right]\psi_{[E]}(\vec{R}_1, \vec{R}_2, \ldots \vec{R}_N) =$$

$$= \left\{-\frac{\hbar^2}{2}\left[m_0^{-1}\frac{\partial^2}{\partial \vec{r}_0^2} + \sum_{\alpha=1}^{N-1}\mu_\alpha\frac{\partial^2}{\partial \vec{r}_\alpha^2}\right] + V(r_1, r_2, \ldots r_{N-1}) - E\right\}\tilde{\psi}_{[E]}(\vec{r}_0, \vec{r}_1, \vec{r}_2, \ldots \vec{r}_{N-1}) = 0$$

must have the certain symmetry in regards to the permutations of all particles. Since the Jacobis' coordinates (2) haven't got the necessary symmetry in regard to the permutations of the particles we have to restore this symmetry later on, in the wave functions by means of the summarizing of the solutions with respect to the permutations of particles. However the dealing with such sums is very difficult and unpractical in most cases.

A quite natural question appears in connection with the fact: whether it is possible to find such a (linear) transformation of the radius-vectors $\vec{R}_i$, so that the new coordinates would be fully symmetrical in regards to the permutations of all particles - (as it analogically takes place for the coordinate of the centre-of-mass of system) - in that case we should work with the right symmetry coordinates from the very beginning. There is a positive answer to the above-mentioned question. It is possible to eliminate the centre-of-mass of N-particle system in such a way that the remaiming part of the classical or quantum-mechanical Hamiltonian is symmetrical in regard to the permutation of all particles. We shall call these coordinates as the generalized symmetrical Jacobis' ones.

The generalized symmetrical Jacobis' coordinates.

In connection with the dealing we mentioned above we are going to introduce the generalized symmetrical Jacobis' coordinates $\vec{r}_0$ and $\vec{r}_\lambda$ ($\lambda = 1,2, \dots N-1$) as the following linear transformation of radius-vectors $\vec{R}_i$:

$$\vec{r}_0 = m_0^{-1} \sum_{i=1}^{N} m_i \vec{R}_i , \quad \vec{r}_\lambda = \sum_{i=1}^{N} e_\lambda^i \vec{R}_i . \qquad (4)$$

The N (N-1) unknown coefficients e_λ^i in (4) are only some non-dimensional functions of the masses of the particles, i.e.

$$e_\lambda^i = e_\lambda^i (m_1, m_2, \dots m_N) .$$

It is well-known that the task of the determination of the coefficients e_λ^i in (4) is **underdetermined** because for N (N-1) coefficients only the $\frac{1}{2}$ N (N-1) conditions exist which we can receive from the form of the transformation of kinetic energy and moment in (1)+/ /3/. To eliminate (or better to restrict) this arbitrariness we shall demand the coefficients e^i_λ to have a certain symmetry in regards to the change of the masses of particles, namely, let the mutual substitution $m_j \leftrightarrow m_k$ in the coefficients e^1_λ, e^2_λ, ... e^N_λ lead to the transformation:

$$e^j_\lambda \leftrightarrow e^k_\lambda \ , \quad e^i_\lambda = \text{const} \ , \quad \text{for} \quad i \neq j,k \ . \tag{5}$$

Substituing the transformation (4) to the formula (3) we receive the $\frac{1}{2}$ N (N+1) following (non-independent) conditions for e^i_λ :

$$\sum_{\lambda=1}^{N-1} \mu_\lambda \, e^i_\lambda \, e^k_\lambda = m_i \, (\delta_{ik} - m_k . \, m_o^{-1}), \ i,k = 1,2 \ldots N. \tag{6}$$

From the conditions (6) by means of their summarizing we may deduce an important relation, namely

$$\sum_{\lambda=1}^{N-1} \mu_\lambda \left(\sum_{i=1}^{N} e^i_\lambda \right)^2 = 0 \ . \tag{7}$$

As all the quantities μ_λ (which represent the masses of some fictious particles) in (7) are positive, hence the (N-1) conditions follow:

$$\sum_{i=1}^{N} e^i_\lambda = 0 \ , \qquad \lambda = 1, 2, \ldots N-1 \tag{8}$$

+/ This arbitrariness is used only when conditions for the usual Jacobis' coordinates with their geometrical meaning are introduced.

The conditions (8) permit us to find the elements of inverse transformation to (4). We signify the determinant of the transformation matrix (4) in terms of Δ , i.e., we put

$$\Delta = m_o^{-1} \cdot \begin{vmatrix} m_1 & m_2 & \cdots & m_N \\ e_1^1 & e_1^2 & \cdots & e_1^N \\ \vdots & \vdots & & \vdots \\ e_{N-1}^1 & e_{N-1}^2 & \cdots & e_{N-1}^N \end{vmatrix} .$$

Since the conditions (8) must be carried out, we remark that all (N-1) x (N-1) **subdeterminants** Δ^i of determinant Δ made up from coefficients e_λ^i can be expressed in terms of Δ , i.e., the following relation holds:

$$\Delta^i = \begin{vmatrix} e_1^1 & \cdots & e_1^{i-1} & e_1^{i+1} & \cdots & e_1^N \\ e_2^1 & \cdots & e_2^{i-1} & e_2^{i+1} & \cdots & e_2^N \\ \vdots & & \vdots & \vdots & & \vdots \\ e_{N-1}^1 & \cdots & e_{N-1}^{i-1} & e_{N-1}^{i+1} & \cdots & e_{N-1}^N \end{vmatrix} = (-1)^{i+1} \; \Delta .$$

On the other hand, the subdeterminants Δ_λ^i obtained from the determinant Δ by cancelling i-th column and $(\lambda+1)$-th row may be expressed in terms of μ_λ, m_i and elements e_λ^i. Indeed, we get:

$$\Delta_\lambda^i = m_o^{-1} \begin{vmatrix} m_1 & m_2 & \cdots & m_{i-1} & m_{i+1} & \cdots & m_N \\ e_1^1 & e_1^2 & \cdots & e_1^{i-1} & e_1^{i+1} & \cdots & e_1^N \\ \cdot & \cdot & & \cdot & \cdot & & \cdot \\ \cdot & \cdot & & \cdot & \cdot & & \cdot \\ \cdot & \cdot & & \cdot & \cdot & & \cdot \\ e_{\lambda-1}^1 & e_{\lambda-1}^2 & \cdots & e_{\lambda-1}^{i-1} & e_{\lambda-1}^{i+1} & & e_{\lambda-1}^N \\ e_{\lambda+1}^1 & e_{\lambda+1}^2 & \cdots & e_{\lambda+1}^{i-1} & e_{\lambda+1}^{i+1} & \cdots & e_{\lambda+1}^N \\ \cdot & \cdot & & \cdot & \cdot & & \cdot \\ \cdot & \cdot & & \cdot & \cdot & & \cdot \\ \cdot & \cdot & & \cdot & \cdot & & \cdot \\ e_{N-1}^1 & e_{N-1}^2 & \cdots & e_{N-1}^{i-1} & e_{N-1}^{i+1} & \cdots & e_{N-1}^N \end{vmatrix} = (-1)^{i+\lambda} \frac{\mu_\lambda}{m_i} e_\lambda^i \, \Delta \qquad (9)$$

The relation (9) may be proved very easily by using the conditions (6). We remark, too, that the determinant Δ^{-1} of the inverse transformation matrix is expressed by means of determinant Δ as

$$\Delta^{-1} = \frac{\mu_1 \, \mu_2 \; \cdots \; \mu_{N-1} \cdot m_o}{m_1 \, m_2 \; \cdots \; m_N} \, \Delta ,$$

and, hence

$$\Delta^2 = \frac{m_1 \cdot m_2 \; \cdots \; m_N}{\mu_1 \cdot \mu_2 \; \cdots \; \mu_{N-1} \cdot m_o} .$$

Having the subdeterminants Δ_λ^i we have as a matter of fact the elements of the inverse transformation matrix.

Therefore, the inverse transformation to (4) is following:

$$\vec{R}_i = \vec{r}_0 + m_i^{-1} \cdot \sum_{\lambda=1}^{N-1} \mu_\lambda \; e_\lambda^i \; \vec{r}_\lambda . \qquad (10)$$

Substituting the expression(10) into the kinetic energy form in (1) we again immediatly find that the following conditions for the coefficients e_λ^i must be satisfied:

$$\sum_{i=1}^{N} e_\lambda^i = 0 , \quad \text{and} \quad \sum_{i=1}^{N} m_i^{-1} e_\lambda^i \; e_\nu^i = \mu_\lambda^{-1} \delta_{\lambda\nu} . \qquad (11)$$

We shall now suppose that the coefficients e_λ^i have the following simple form:

$$e_\lambda^i = \frac{A_\lambda}{\alpha_\lambda - a_i} , \qquad (12)$$

where the parameters $a_i = m_i^{-1}$ (inverse masses), and 2 (N-1) unknown quantities A_λ and α_λ are some symmetrical functions of the parameters $a_1, a_2, \ldots a_N$, i.c.,masses of all particles. The simple form of the coefficients in (12) possesses all the necessary properties given in (5) in regards to the permutations of all N particles. The quantities A_λ and α_λ must be determined from those conditions which also satisfy the coefficients e_λ^i .

First of all, the coefficients e_λ^i must satisfy conditions (8) and, therefore the following must holds:

$$\sum_{i=1}^{N} e_{\lambda}^{i} = A_{\lambda} \sum_{i=1}^{N} (\alpha_{\lambda} - a_i)^{-1} = A_{\lambda} P'_N(\alpha_{\lambda}) \left[P_N(\alpha_{\lambda}) \right]^{-1} = 0,$$

where we introduced the notation $P_N(\alpha)$ for a polynomial of the N - th degree

$$P_N(\alpha) = \sum_{i=1}^{N} (\alpha - a_i) = \sum_{k=o}^{N} (-1)^k g_k \alpha^{N-k} \qquad (13)$$

and $P'_N(\alpha)$ is the first derivation with respect to α of $P_N(\alpha)$, i.e.,

$$P'_N(\alpha) = \frac{d}{d\alpha} \sum_{i=1}^{N} (\alpha - a_i) = P_N(\alpha) \sum_{i=1}^{N} (\alpha - a_i)^{-1} =$$

$$= \sum_{k=0}^{N-1} (-1)^k (N-k) g_k \alpha^{N-k-1} .$$

The quantities g_k ($g_o = 1$) in (13) are the elementary algebraic symmetrical polymonials made up from the parameters $a_1, a_2, \dots a_N$.

If we now put

$$P'_N(\alpha) = 0 \qquad (14)$$

the conditions (8) are fulfilled. We designate the roots of the algebraic equation (14) of (N-1) degree in terms of $\alpha_1, \alpha_2, \dots \alpha_{N-1}$. It is easy to show that for the case of all different masses all the roots α_{λ} are real, positive and different, where the following relations hold:

$a_1 \leq \alpha_1 \leq a_2 \leq \alpha_2 \leq \dots \alpha_{N-1} \leq a_N$. In addition the second conditions in (11) for $\lambda \neq \nu$ may be rewritten in the following form.

$$\sum_{i=1}^{N} a_i \; e^i_\lambda \; e^i_\nu = A_\lambda \; A_\nu \sum_{i=1}^{N} a_i \left[(\alpha_\lambda - a_i) \; (\alpha_\nu - a_i) \right]^{-1} =$$

$$= A_\lambda \; A_\nu \; (\alpha_\lambda - \alpha_\nu)^{-1} \left[\alpha_\lambda P'_N \; (\alpha_\lambda) - \alpha_\nu P_N \; (\alpha_\nu) \right] = 0$$

and it is clear that they are fulfilled automatically. On the other hand, for $\lambda = \nu$ from the second conditions in (11) we obtain:

$$\mu_\lambda^{-1} = \sum_{i=1}^{N} a_i \; (e^i_\lambda)^2 = A^2_\lambda \sum_{i=1}^{N} a_i \; (\alpha_\lambda - a_i)^{-2} = \tag{15}$$

$$= - A^2_\lambda \alpha_\lambda \left\{ P''_N (\alpha_\lambda) \; [P_N \; (\alpha_\lambda)]^{-1} + [P'_N \; (\alpha_\lambda)]^2 \; [P_N \; (\alpha_\lambda)]^{-2} \right\},$$

where $P''_N (\alpha)$ is the second derivation of $P_N (\alpha)$ with respect to α. Since $P'_N \; (\alpha) = 0$ the relation (15) determines the unknown quantities A_λ which are equal to the following expression:

$$A_\lambda = \pm \left[- \frac{P_N \; (\alpha_\lambda)}{\mu_\lambda \; \alpha_\lambda \; P''_N \; (\alpha_\lambda)} \right]^{\frac{1}{2}} . \tag{16}$$

The sign before the square root in (16) has no meaning and for the definiteness we choose the positive one. Thus, we have determined A_λ and α_λ in the coefficients e^i_λ in (12) by means of (14) and (16), and we can write them in the following explicit form:

$$e_\lambda^i = \mathrm{sign}\,(\alpha_\lambda - a_i)\left[-\frac{P_N(\alpha_\lambda)}{\mu_\lambda\alpha_\lambda(\alpha_\lambda - a_i)^2 P_N''(\alpha_\lambda)}\right]^{\frac{1}{2}} . \qquad (17)$$

The coefficients e_λ^i in the form (17) contain the masses μ_λ which were undetermined till now. These masses however cannot be determined from the form of the kinetic energy in (4). For the determination of masses μ_λ we must make use of some other conditions following (for example) from the concrete form of the potential $V(\vec{r}_1, \vec{r}_2 \ldots \vec{r}_{N-1})$. Without loss of generality we can suppose for convenience, all masses are equal, i.e.,

$$\mu_1 = \mu_2 = \ldots \mu_{N-1} = \left[m_1 m_2 \ldots m_N \, m_0^{-1} \, \Delta^{-2} \right]^{\frac{1}{N-1}} .$$

There is also some other way to receive the simple connection between μ_λ and α_λ. The lengths of the vectors $\vec{r}_\lambda$ in (4) are arbitrary and we can „normalize" them by means of normalizing the lengths of the vectors with the components $e_\lambda^1, e_\lambda^2, \ldots e_\lambda^N$. Using the relations mentioned above we have for $\lambda \neq \nu$:

$$\sum_{i=1}^{N} e_\lambda^i \, e_\nu^i = A_\lambda \, A_\nu \, (\alpha_\lambda - \alpha_\nu)^{-1} \, [P_N'(\alpha_\lambda) - P_N(\alpha_\nu)] = 0 ,$$

and also for $\lambda = \nu$:

$$\sum_{i=1}^{N} (e_\lambda^i)^2 = A_\lambda^2 \sum_{i=1}^{N} (\alpha_\lambda - a_i)^{-2} = (\alpha_\lambda \mu_\lambda)^{-1}$$

so that we can write:

$$\sum_{i=1}^{N} e_{\lambda}^{i} \; e_{\nu}^{i} = (\alpha_{\lambda}\mu_{\lambda})^{-1} \delta_{\lambda\nu} . \qquad (18)$$

If we choose the normalization in (18) equal to one, we have $\alpha_{\lambda}\mu_{\lambda} = 1$, i.e., $\mu_{\lambda} = \alpha_{\lambda}^{-1}$. Thus, in the given case we received a simple connection of the fictive masses μ_{λ} in terms of the masses m_i . However it should be noted once again that such choice of the normalization is not obligate and the dependence μ_{λ} on m_i is determined by the concrete physical problem.

Finally we also note that the form of the moment $\vec{M}_o$ of the N-particle system in (1) can be easily expressed by means of the generalized symmetrical Jacobis' coordinates (4), too, in the following way:

$$\vec{M}_o = \sum_{i=1}^{N} m_i \, [\vec{R}_i \times \dot{\vec{R}}_i] = m_o \, [\vec{r}_o \times \dot{\vec{r}}_o] + \sum_{\lambda=1}^{N-1} \mu_{\lambda} \, [\vec{r}_{\lambda} \times \dot{\vec{r}}_{\lambda}] .$$

C o n c l u s i o n

The problem formulated in the beginning is solved. The Jacobis' coordinates having the necessary properties with respect to the permutations are found. The introduction of the generalized symmetrical Jacobis' coordinates (4) does not solve, of course, still yet the problem of the N interacting particles; it solves only the particular problem of the N free particles. The solution of such a problem is also of great importance, first of all,in the quantum mechanics,where the solutions of many-particle Schrödinger's equation must have a certain parity in regards to the permutations of the particles.

Note shall be taken to the particular cases of the introduced Jacobis' coordinates, when two (or more) masses are equal. In this case our coordinates for N particle system reduce to the coordinates of the analogic type but with a less number of particles. The form of the reduced coordinates depends on the sequence of the limited transitions in the system. The explicit form of the symmetrical Jacobis' coordinates for N = 3 is considered in paper[5].

The symmetrical elimination of the centre-of-mass of N particle system allows one to formulate a whole series of new and interesting problems. For example we can easily convince that the following formula holds

$$\frac{1}{2} m_0^{-1} \sum_{i,k=1}^{N} m_i m_k (\vec{R}_i - \vec{R}_k)^2 = \sum_{\lambda=1}^{N-1} \mu_\lambda \vec{r}_\lambda^{\,2} .$$

It means that the quantum-mechanical problem with a harmonic oscillator type potential can be solved completely. There are some other potentials being of interest from the physical point of view which permit the total solution of equations of the motion. It is known that in the nuclear physics the method of K - harmonics is worked out. Basing on the generalized symmetrical Jacobis' coordinates we can construct K-harmonics, too, and these K-harmonics will possess the useful properties with respect to the permutations of the particles. These and some other problems will be worked out in the future.

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