acta phys. slov. 23 (1973), No. 2

A COMPLETE SET OF FUNCTIONS IN THE QUANTUM MECHANICAL THREE-BODY PROBLEM[1]

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A complete set of basis functions for the quantum mechanical three-body problem is chosen in the form of hyperspherical functions. These functions are characterized by quantum numbers corresponding to the chain O(6) ⊃ SU(3) ⊃ O(3). Equations are derived to obtain the basis functions in an explicit form.

I. INTRODUCTION

Elementary processes involving three interacting particles exhibit an extremely complicated structure. It is therefore important to have at least a complete understanding of systems consisting of non-interacting particles. These non-interacting states form a complete set of basis vectors, in terms of which the wave functions of interacting particles can be expanded.

In any classification of multiparticle states it is important to diagonalize those variables which are known to be constants of motion from general invariance principles; one usually takes the total energy and angular momentum. In nuclear physics we deal with particles of equal or nearly equal masses; evidently, it would be useful to have a method for constructing multiparticle angular momentum states which treat all particles on an equal footing.

The aim of the present paper is to find a complete set of orthonormal functions, corresponding to three free particles. Doing so, we introduce hyperspherical functions, i.e. functions, which are defined on the five-dimensional sphere, and are eigenfunctions of the angular part of the six-dimensional Laplacian. They have to describe states with given angular momenta and definite permutation symmetry properties. This choice of functions is due to the invariance of the free Hamiltonian under the O(6) or SU(3) group.

[1] Talk given at Elementary Particle Physics Seminar at Pezinská Baba, September 22–25, 1971.

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The group-theoretical features of the three-particle states which follow from this invariance were studied by several authors [1–10]. The classification of the three-particle states based on these groups according to the chain O(6) ⊃ ⊃ SU(3) ⊃ O(3) gives 4 quantum numbers, namely: K — the six-dimensional momentum, corresponding to the eigenvalue of the six-dimensional Laplacian; J — the angular momentum and its projection M, and a number ν, which characterizes the permutation symmetry. On the other hand, the motion of a system of n particles in a given energy and momentum state can be defined by $3n$-4 parameters, and requires for its quantum-mechanical description $3n$-4 quantum numbers, i.e. five in the case of three particles. That means that the states labelled according to the chain above might be degenerate; this degeneracy can be eliminated either by the straightforward orthogonalization of the functions, or with help of a hermitian operator $\hat{\Omega}$, which we take from the group O(6), and which commutes with the O(3) generators. The eigenvalue of this operator is the fifth — missing — quantum number Ω. Unfortunately, since $\hat{\Omega}$ is a cubic operator, it leads to rather complicated eigenvalue equations.

II. GROUP-THEORETICAL PROPERTIES. CHOICE OF COORDINATES AND PARAMETRIZATION

In the present paper we first make an attempt to calculate directly the eigenfunctions corresponding to the given five quantum numbers K, J, M, ν, Ω. If one intends to construct harmonic functions for the three-particle system analogous to the spherical functions forming the basis in the case of two particles, it is natural to use angular variables on the five-dimensional sphere, and build up the wanted functions in terms of these coordinates. First of all, it is essential to take the proper parametrization. We will consider particles with equal masses. Let $\vec{x}_i$ $(i = 1, 2, 3)$ be the radius-vectors of the three particles, and fix them by the condition $\vec{x}_1 + \vec{x}_2 + x_3 = 0$. The Jacobi-coordinates will be defined as

$$\vec{\xi} = -(3/2)^{1/2}(\vec{x}_1 + \vec{x}_2); \quad \vec{\eta} = (2)^{-1/2}(\vec{x}_1 - \vec{x}_2)$$

$$\xi^2 + \eta^2 = \varrho^2 = x_1^2 + x_2^2 + x_3^2,$$

where ϱ is the radius of the 5-sphere. The permutations mix up the components of $\vec{\xi}$ and $\vec{\eta}$, and therefore it is useful to consider a 6-vector $\begin{pmatrix}\xi\\ \eta\end{pmatrix}$, for which we have

$$P_{12}\begin{pmatrix}\xi\\ \eta\end{pmatrix} = \begin{pmatrix}\xi\\ -\eta\end{pmatrix}$$

$$P_{13}\begin{pmatrix}\xi\\ \eta\end{pmatrix} = \begin{pmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & \frac{1}{2} \end{pmatrix}\begin{pmatrix}\xi\\ \eta\end{pmatrix}, \quad P_{23}\begin{pmatrix}\xi\\ \eta\end{pmatrix} = \begin{pmatrix} -\frac{1}{2} & \frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & \frac{1}{2} \end{pmatrix}\begin{pmatrix}\xi\\ \eta\end{pmatrix}.$$

Thus the permutations appear as some rotations in the 6-dimensional space; $\varrho^2 = \xi^2 + \eta^2$ can be considered as the invariant of O(6).

Further, we introduce the complex vectors

$$\vec{z} = \vec{\xi} + i\vec{\eta}$$
$$\vec{z}^* = \vec{\xi} - i\vec{\eta}.$$

For them the permutation symmetry properties are especially simple:

$$P_{12}\, z = z^*, \quad P_{13}\, z = z^*\, e^{-\frac{2}{3}\pi i}, \quad P_{23}\, z = z^*\, e^{\frac{2}{3}\pi i}$$
$$P_{12}\, z^* = z, \quad P_{13}\, z^* = z\, e^{\frac{2}{3}\pi i}, \quad P_{23}\, z^* = z\, e^{-\frac{2}{3}\pi i}.$$

On these vectors one can build up the group SU(3), the condition $\xi^2 + \eta^2 = |z|^2 = \varrho^2$ gives its invariant.

In order to complete the parametrization, let us consider a triangle, the vertices of which are given by three particles. The situation of this triangle in space will be determined by the unit vectors $\vec{l}_1$, $\vec{l}_2$ which, together with $\vec{l} = \vec{l}_1 \times \vec{l}_2$, form the moving coordinate system. Their orientation towards the fixed system of coordinates is described by the Euler angles. The vectors $\vec{l}_1$ and $\vec{l}_2$ are connected with z in the following way:

$$\vec{z} = 2^{-1/2}\varrho\, e^{-i(\lambda/2)}\, (e^{i(a/2)}\, \vec{l}_1 + i e^{-i(a/2)}\, \vec{l}_2).$$

The parameters λ and a characterize the form of the triangle (except the similarity transformations, which we can exclude putting $\varrho = \text{const.}$). Note that the parametrization is chosen in such a way that

$$\vec{l}_m k_n = l_m^{(n)} = D^1_{mn}(\varphi_1 \ominus \varphi_2)$$

and

$$z_m = \sum_{\mu=\pm 1} D^{1/2}_{1/2-\mu/2}(\lambda, a, 0)\, D^1_{-\mu,m}(\varphi_1 \ominus \varphi_2),$$

i.e. we can separate explicitely the rotations and the deformations of the triangle. ($\vec{l}_m$ and $\vec{k}_n$ are unit vectors corresponding to the moving and the fixed coordinate systems, respectively.)

III. GENERATORS AND CASIMIR OPERATORS, EIGENFUNCTIONS

Now we can calculate the operators, the eigenvalues of which we are trying to find. They are:

$$\Delta = |A_{ik}|^2,$$

the Laplace operator on the five-dimensional sphere; here

$$A_{ik} = i z_i \frac{\partial}{\partial z_k} - i z_k^* \frac{\partial}{\partial z_i^*} \text{ are the SU(3) generators;}$$

$$J_{ik} = \tfrac{1}{2}(A_{ik} - A_{ki}) = \tfrac{1}{2}\left(i z_i \frac{\partial}{\partial z_k} - i z_k \frac{\partial}{\partial z_i} + i z_i^* \frac{\partial}{\partial z_k^*} - i z_k^* \frac{\partial}{\partial z_i^*}\right),$$

the generator of the three-dimensional rotation group; the scalar operator

$$N = \tfrac{1}{2} \sum_k \left(z_k \frac{\partial}{\partial z_k} - z_k^* \frac{\partial}{\partial z_k^*}\right) = \frac{1}{2i}\, \mathrm{Sp}\, A,$$

the eigenvalue of which is ν, and finally the operator

$$\hat{\Omega} = \sum_{i,k,l} J_{ik}\, B_{kl} J_{li},$$

where

$$B_{ik} = \tfrac{1}{2}(A_{ik} + A_{ki}) = \tfrac{1}{2}\left(i z_i \frac{\partial}{\partial z_k} + i z_k \frac{\partial}{\partial z_i} - i z_i^* \frac{\partial}{\partial z_k^*} - i z_k^* \frac{\partial}{\partial z_i^*}\right)$$

is the generator of the group of deformations of the triangle.

The explicit expressions for these five commuting operators are the following. Using

$$ds^2 = |dz|^2 = g_{ik} q^i q^k = \varrho^2[\tfrac{1}{4}\, da^2 + \tfrac{1}{4}\, d\lambda^2 + \tfrac{1}{2}\, d\Omega_1^2 + \tfrac{1}{2}\, d\Omega_2^2 +$$
$$+ d\Omega_3^2 - \sin a\, d\Omega_1 d\Omega_2 - \cos a\, d\Omega_3 d\lambda] + d\varrho^2,$$

where $d\Omega_i$ are infinitesimal rotations about the moving axes, we obtain the Laplacian:

$$\Delta = g^{-1/2} \frac{\partial}{\partial q^i}\, g^{ik}\, g^{1/2} \frac{\partial}{\partial q^k} =$$

$$= 4\left\{\frac{\partial}{\partial a^2} + 2\mathrm{ctg}\, 2a \frac{\partial}{\partial a} + \frac{1}{\sin^2 a}\left(\frac{\partial^2}{\partial \lambda^2} + \cos a \frac{\partial^2}{\partial \lambda \partial \Omega_3} + \frac{1}{4}\frac{\partial^2}{\partial \Omega_3^2}\right) + \right.$$

$$+\frac{1}{2\cos^2 a}\left[\frac{\partial^2}{\partial\Omega_1^2}+\sin a\left(\frac{\partial^2}{\partial\Omega_1\partial\Omega_2}+\frac{\partial^2}{\partial\Omega_2\partial\Omega_1}\right)+\frac{\partial^2}{\partial\Omega_2^2}\right]\Bigg\}.$$

The explicit form of N is $N = \mathrm{i}\frac{\partial}{\partial\lambda}$. If a harmonic function Φ is an eigenfunction of Δ, it has to fulfil

$$\Delta\Phi = -K(K+4)\,\Phi$$

and

$$N\Phi = \nu\Phi.$$

(We remark here that if the harmonic function belongs to the SU(3) representation (p, q), then $K = p + q$, $\nu = \frac{1}{2}(p - q)$.)

The operator J_{ik} is obtained in the form

$$J_{ik} = -\frac{\mathrm{i}}{2}\,\varepsilon_{ikl}\left[l_1^{(1)}\frac{\partial}{\partial\Omega_1}+l_2^{(1)}\frac{\partial}{\partial\Omega_2}+l^{(1)}\frac{\partial}{\partial\Omega_3}\right].$$

Finally we get

$$\hat{\Omega} = -\frac{1}{4}\Bigg\{2^{1/2}\left(\frac{\partial^2}{\partial\Omega_+^2}H_+ + \frac{\partial^2}{\partial\Omega_-^2}H_-\right)+\frac{\partial^2}{\partial\Omega_3^2}\frac{\partial}{\partial\lambda}+\Delta\ominus\frac{\partial}{\partial\lambda}-$$
$$-\frac{1}{\cos a}\left(\Delta\ominus-\frac{\partial^2}{\partial\Omega_3^2}+\frac{1}{2}\right)\frac{\partial}{\partial\Omega_3}+$$
$$+\operatorname{tg} a\left[\mathrm{i}\left(\frac{\partial^2}{\partial\Omega_+^2}-\frac{\partial^2}{\partial\Omega_-^2}\right)\frac{\partial}{\partial\Omega_3}-\frac{3}{2}\left(\frac{\partial^2}{\partial\Omega_+^2}+\frac{\partial^2}{\partial\Omega_-^2}\right)\right]\Bigg\},$$

where

$$H_\pm = 2^{-1/2}\left[\frac{\partial}{\partial a}\pm\mathrm{i}\frac{1}{\sin a}\frac{\partial}{\partial\lambda}\pm\frac{\mathrm{i}}{2}\operatorname{ctg} a\frac{\partial}{\partial\Omega_3}\right]$$
$$\frac{\partial}{\partial\Omega_\pm} = 2^{-1/2}\left(\frac{\partial}{\partial\Omega_1}\pm\mathrm{i}\frac{\partial}{\partial\Omega_2}\right).$$

Before writing down the eigenfunctions of these five operators, we have to make a few remarks. One can show that for $K < 4$ all states are simple; in the interval $4 \leq K < 8$ doubly degenerated states show up; and so on, n-fold degeneration appears at the value $K = 4n$. Besides, states with $J = 0$ and $J = K$ values are not degenerated. Consequently for practical purposes it is enough to deal with four quantum numbers.

Finally, let us look for the harmonic functions Φ which fulfil the eigenvalue equations of the Laplace operator and the operator N with eigenvalues $K(K+4)$ and ν, respectively. The general form is the following:

$$\Phi^J_{M,\nu} = \sum_\varkappa\sum_\mu a_\nu(\varkappa,\mu)\,D^{(K/2)-\varkappa}_{\nu,(\mu/2)}(\lambda, a, 0)\,D^J_{\mu,M}(\varphi_1\ominus\varphi_2).$$

It is easy to understand the meaning of this solution. One can consider the second D-function — which is the eigenfunction of J^2 and J_3 — as an eigenfunction of a rotating rigid top with the projection of angular momentum on the moving axis equal to μ. This projection is not conserved in our case, that is why we have to sum over different values of μ. That is just the point where we need an additional operator to orthogonalize the obtained functions. The coefficients $a_\nu(\varkappa,\mu)$ have to be defined from the equations

$$\Delta\Phi^J_{M,\nu} = -K(K+4)\,\Phi^J_{M,\nu}$$

and

$$\hat{\Omega}\Phi^J_{M,\nu} = \Omega\Phi^J_{M,\nu}.$$

These equations are unfortunately somewhat complicated:

$$\sum_\varkappa\sum_\mu\Bigg\{\Bigg[a_\nu(\varkappa,\mu-2)\frac{1}{2}\sqrt{\left(\frac{K}{2}-\frac{\mu}{2}-\varkappa+1\right)\left(\frac{K}{2}+\frac{\mu}{2}-\varkappa\right)}\times$$
$$\times\sqrt{(J-\mu+2)(J-\mu+1)(J+\mu-1)(J+\mu)}+a_\nu(\varkappa,\mu+2)\frac{1}{2}\times$$
$$\times\sqrt{\left(\frac{K}{2}+\frac{\mu}{2}-\varkappa+1\right)\left(\frac{K}{2}-\frac{\mu}{2}-\varkappa\right)}\sqrt{(J+\mu+2)(J+\mu+1)(J-\mu-1)(J-\mu)}+$$
$$+a_\nu(\varkappa,\mu)(\nu\mu^2+J(J+1)\nu-4\mathrm{i}\Omega)\Bigg]D^{K/2-\varkappa}_{\nu,(\mu/2)}(\lambda,a,0)\,D^J_{\mu,M}(\varphi_1\ominus\varphi_2)+a_\nu(\varkappa,\mu)\times$$
$$\times\left[\frac{\mu}{\cos a}\left(J(J+1)-\mu^2+\frac{1}{2}\right)D^{K/2-\varkappa}_{\nu,(\mu/2)}(\lambda,a,0)\,D^J_{\mu,M}(\varphi_1\ominus\varphi_2)+\mathrm{i}\operatorname{tg} a\times\right.$$
$$\times\left(\left(\frac{\mu}{2}+\frac{3}{4}\right)\sqrt{(J-\mu)(J+\mu+1)(J-\mu-1)(J+\mu+2)}\,D^{K/2-\varkappa}_{\nu,(\mu/2)}(\lambda,a,0)\times\right.$$
$$\times D^J_{\mu+2,M}(\varphi_1\ominus\varphi_2)-\left(\frac{\mu}{2}-\frac{3}{4}\right)\sqrt{(J+\mu)(J-\mu+1)(J+\mu-1)(J-\mu+2)}\times$$

$$\times D^{K/2-\varkappa}_{\nu,(\mu/2)}(\lambda, a, 0)\, D^J_{\mu-2,M}(\varphi_1 \ominus \varphi_2)\Big)\Big]\Big\} = 0$$

and

$$\sum_{\varkappa}\sum_{\mu}\Big\{a_\nu(\varkappa,\mu)\Big[-\Big(\frac{K}{2}-\varkappa\Big)\Big(\frac{K}{2}-\varkappa+1\Big)+\frac{1}{4}K(K+4)-\frac{\mu}{2}+\frac{\nu}{\cos a}-$$

$$-\frac{1}{2\cos^2 a}J(J+1)+\frac{\mu^2}{2\cos^2 a}\Big]\, D^{K/2-\varkappa}_{\nu,(\mu/2)}(\lambda, a, 0)\, D^J_{\mu,M}(\varphi_1 \ominus \varphi_2) -$$

$$-a_\nu(\varkappa, \mu-2)\,\mathrm{i}\,\mathrm{tg}\, a\sqrt{\Big(\frac{K}{2}-\frac{\mu}{2}-\varkappa+1\Big)\Big(\frac{K}{2}+\frac{\mu}{2}-\varkappa\Big)}\, D^{K/2-\varkappa}_{\nu,(\mu/2)}(\lambda, a, 0)\times$$

$$\times D^J_{\mu-2,M}(\varphi_1 \ominus \varphi_2) + a_\nu(\varkappa,\mu)\Big[-\frac{\mathrm{i}\sin a}{4\cos^2 a}\times$$

$$\times\sqrt{(J-\mu)(J+\mu+1)(J-\mu-1)(J+\mu+2)}\times$$

$$\times D^{K/2-\varkappa}_{\nu,(\mu/2)}(\lambda, a, 0) D^J_{\mu+2,M}(\varphi_1\ominus\varphi_2)+\frac{\mathrm{i}\sin a}{4\cos^2 a}\times$$

$$\times\sqrt{(J+\mu)(J-\mu+1)(J+\mu-1)(J-\mu+2)}\, D^{K/2-\varkappa}_{\nu,(\mu/2)}(\lambda, a, 0)\, D^J_{\mu-2,M}(\varphi_1\ominus\varphi_2)\Big]\Big\} = 0$$

and, although it es quite easy to solve this set of equations for every particular case, we have not been able so far to obtain a general solution.

IV. ANOTHER WAY OF CONSTRUCTING A SET OF EIGENFUNCTIONS

There is another way to find this complete set of functions. In fact, the problem becomes complicated because of the requirement of definite permutation symmetry properties. Without them it would be simple to construct the wanted functions with the help of the graphical method of the so-called "tree-functions" [17], which was proposed by Vilenkin and Smorodinsky. We have to modify these functions, i.e. we have to find a transformation from the complete set of "tree-functions" to the K-harmonics. (K-harmonics are hyperspherical functions possessing definite permutation symmetry properties.) Thus we first construct the "tree-functions", which are characterized by quantum numbers

$$K, j_1, M_1, j_2, M_2$$

(j_1, M_1 and j_2, M_2 are angular momenta and their projections conjugated to $\vec{\xi}$ and $\vec{\eta}$). We have to trasform these functions to a set of K-harmonics, which is described by the quantum numbers K, J, M, ν, $(j_1 j_2)$. In order to do this it is necessary to carry out a simple Fourier transform. To be correct, $(j_1 j_2)$ is not a real quantum number in the sense that functions corresponding to different pairs $(j_1 j_2)$ do not form an orthonormal set, but this notation demonstrates where we get these functions from. Their explicit expression is the following:

$$\Phi^{j_1 j_2}_{JM\nu}(\vec{\xi}, \vec{\eta}) = A_{JM}\sum_m\sum_{\mu,\delta}\sum_{\varkappa}\Big(j_1, \frac{\mu+\delta}{2}; j_2, \frac{\mu-\delta}{2}\Big| J; \mu\Big)^2\times$$

$$\times\frac{\begin{pmatrix}\frac{K-\delta}{4}, & W+\frac{\mu}{4}; & \frac{K+\delta}{4}, & -W+\frac{\mu}{4} & \Big| & \frac{K}{2}-\varkappa; & \frac{\mu}{2}\end{pmatrix}}{\begin{pmatrix}\frac{j_1}{2}+m, & \frac{\mu+\delta}{4}; & \frac{j_2}{2}+n-m, & \frac{\mu-\delta}{4} & \Big| & \frac{K}{2}; & \frac{\mu}{2}\end{pmatrix}}\,\frac{(-1)^{\frac{K+\mu-\delta}{4}-\frac{\nu}{2}+\varkappa}}{2^{K/4}}\times$$

$$\times\frac{\Delta^{(J)}_{0\mu}\Delta^{((K/2)-\varkappa)}_{\delta/2,\nu}}{\Delta^{(K/2)}_{K/2,\mu/2}}\Big[\frac{(j_1+2m)!\,(j_2+2n-2m)!}{(K+\varkappa+1)!\,\varkappa!}\Big]^{1/2}\binom{n+j_1+\frac12}{m}\binom{n+j_2+\frac12}{n-m}\times$$

$$\times D^{(K/2)-\varkappa}_{\nu,\mu/2}(\lambda, a, 0)\, D^J_{\mu,M}(\varphi_1\ominus\varphi_2)$$

where A_{JM} consists of norming constants and Clebsch-Gordan coefficients.

The solutions of the eigenvalue equations for K and Ω have to be linear combinations of these functions:

$$\Phi^J_{M,\nu} = \sum_{j_1 j_2} c_{(j_1 j_2)}\,\Phi^{j_1 j_2}_{JM\nu}(\vec{\xi}, \vec{\eta}),$$

where $(j_1 j_2)$ will run over each pair of values which can give the total angular momentum J such that

$$J \le j_1 + j_2 \le K.$$

Looking at the structure of the coefficient, it is easy to understand that our attempt to determine $a_\nu(\varkappa, \mu)$ directly could not be successful.

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Received September 22nd, 1971