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Construction of the hyperspherical functions for the quantum mechanics of three particles

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Abstract. A solution of the differential equation for the grand angular momentum in hyperspherical coordinates is given by simple algebraic means avoiding complicated recurrence formulae.

1. Introduction

In recent years, a new approach has been made to the quantum mechanical three-body problem, using hyperspherical functions which form simultaneously a representation of the groups of three-dimensional space rotations and of the permutations of three particles. Some of the authors who have tried to carry through this general idea have emphasized its group theoretical side, and some have tried to solve explicitly the Schrödinger equation for the special case of three free particles.

Dragt (1965) and Simonov (1966) laid the foundations to the group theoretical approach of constructing the hyperspherical functions which constitute a complete orthogonal set on the unit sphere in six-dimensional space. Their results, however, valuable for the principal understanding of the problem, turned out to be rather tedious for practical use, even for small values of angular momentum J. On the other hand, Zickendraht (1965) started from the Schrödinger equation and found functions up to total angular momentum $J = 2$, but the coordinates used are unusual in the theory of hyperspherical functions. Whitten and Smith (1968) started from the same point of view but their method becomes very cumbersome even for small values of grand angular momentum K (where $J \leqslant K$). Hyperspherical functions are given up to $K = 4$ but no generalization has been obtained for higher values of K or J.

In the present paper we also follow the way of directly solving the Schrödinger equation of three free particles, making extensive use of the results of the authors quoted above to whom we refer the reader for details. In § 2 of this paper we introduce the coordinates and the basic differential equation for the operator Λ^2 of grand angular momentum,

$$\Lambda^2 F = K(K+4)F \tag{1}$$

in these coordinates, following from the Schrödinger equation. In § 3 the method will be developed, for any given angular momentum J, to obtain the complete set of linearly independent solutions of (1). Since it will be necessary to distinguish between the cases of $J+K$ even or odd, and another quantum number $\nu \geqslant 0$ or $\nu < 0$, the method is explained in detail only for $J+K$ even and $\nu \geqslant 0$; formulae for the other cases are only summarized in the appendix.

2. The hyperspherical coordinates

We shall use in position space of any three particles essentially the same coordinates which Dragt (1965) has introduced in momentum space for three equal masses. Let m_i ($i = 1, 2, 3$) be the masses and $\boldsymbol{r}_i$ the position vectors of the three particles; we then define relative coordinates

$$\begin{aligned} \boldsymbol{x}_1 &= \boldsymbol{r}_2 - \boldsymbol{r}_1 \\ \boldsymbol{x}_2 &= \boldsymbol{r}_3 - \frac{m_1\boldsymbol{r}_1 + m_2\boldsymbol{r}_2}{m_1 + m_2} \\ \boldsymbol{R} &= \frac{m_1\boldsymbol{r}_1 + m_2\boldsymbol{r}_2 + m_3\boldsymbol{r}_3}{m_1 + m_2 + m_3}. \end{aligned} \tag{2}$$

Three external coordinates are defined by the Euler angles α, β, γ describing a rotation from space-fixed axes in the centre of mass system into body-fixed axes $\boldsymbol{y}_1, \boldsymbol{y}_2$ and $\boldsymbol{y}_1 \times \boldsymbol{y}_2$ which make the tensor of inertia diagonal. The convention of Euler angles and rotation matrices D^J_{MN} and d^J_{MN} is the same as in Rose (1967). Thus the directions of $\boldsymbol{y}_1$ and $\boldsymbol{y}_2$ coincide with the principal moments of inertia in the plane of the three particles. With the three moments of inertia kept fixed, the vectors $\boldsymbol{x}_1$ and $\boldsymbol{x}_2$ in the body-fixed system are connected with $\boldsymbol{y}_1$ and $\boldsymbol{y}_2$ by a so called kinematic rotation (Smith 1960)

$$\begin{aligned} \boldsymbol{x}_1 &= \boldsymbol{y}_1 \sin\tfrac{1}{2}\varphi - \boldsymbol{y}_2 \cos\tfrac{1}{2}\varphi \\ \boldsymbol{x}_2 &= \boldsymbol{y}_1 \cos\tfrac{1}{2}\varphi + \boldsymbol{y}_2 \sin\tfrac{1}{2}\varphi. \end{aligned} \tag{3}$$

In the plane of three particles in the body-fixed system we define three internal coordinates. Two of them are connected with the moments of inertia. The hyperradius r is defined by

$$\mu r^2 = m_1 r_1^2 + m_2 r_2^2 + m_3 r_3^2 \tag{4}$$

with

$$\mu = \frac{9 m_1 m_2 m_3}{(m_1 + m_2 + m_3)^2}. \tag{5}$$

r is connected with the moment of inertia with respect to an axis perpendicular to the plane of the three particles

$$\theta_{zz} = \mu r^2. \tag{6}$$

The second internal coordinate ψ gives the other two momenta

$$\begin{aligned} \theta_{xx} &= \mu r^2 \sin^2\psi \\ \theta_{yy} &= \mu r^2 \cos^2\psi. \end{aligned} \tag{7}$$

The third coordinate is the angle φ, which describes the different positions the three particles can have once the three moments of inertia are fixed.

It is helpful to illustrate the three coordinates in the case of three equal particles. Figure 1 shows that the hyperradius r is a measure of the spatial extension of the ellipse on which the particles lie. For $\psi = \pi/4$ the ellipse becomes a circle and for $\psi = 0$ the

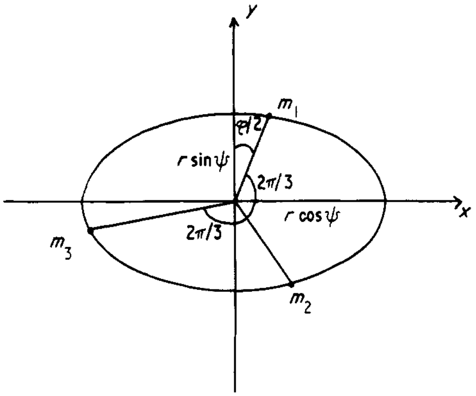

Figure 1. Relative location of the three particles for three equal masses.

three particles lie on the x axis. For $\pi/4 \leqslant \psi \leqslant \pi/2$ we also get an ellipse, and by interchanging the x and y axes, ie another set of Euler angles, we always have

$$\theta_{xx} \leqslant \theta_{yy} \leqslant \theta_{zz}. \tag{8}$$

The same argument holds for $\varphi \geqslant 2\pi$, so that the ranges of definition for ψ and φ are

$$\begin{aligned} &0 \leqslant \psi \leqslant \pi/4 \\ &0 \leqslant \varphi \leqslant 2\pi. \end{aligned} \tag{9}$$

In terms of the new coordinates we now get the position vectors $\boldsymbol{r}_i$ in the space-fixed system:

$$\boldsymbol{r}_i = 3\frac{m_j+m_k}{M}\left(\frac{\mu_{jk}}{M}\right)^{1/2} \mathscr{M}^{-1}(\alpha, \beta, \gamma) r \begin{pmatrix} \cos\psi & \cos(\frac{1}{2}\varphi+\beta_i) \\ \sin\psi & \sin(\frac{1}{2}\varphi+\beta_i) \\ & 0 \end{pmatrix} + \boldsymbol{R} \tag{10}$$

where

$$M = m_1+m_2+m_3, \qquad \mu_{jk} = \frac{m_j m_k}{m_j+m_k}$$

and $\mathscr{M}^{-1}(\alpha, \beta, \gamma) = \mathscr{M}(-\gamma, -\beta, -\alpha)$ is the matrix describing the coordinate rotation (cf Rose 1967, p 65).

The angles β_i are constants connected with the three masses,

$$\begin{aligned} \cos\beta_1 &= -\left(\frac{m_1 m_3}{(m_1+m_2)(m_2+m_3)}\right)^{1/2}, \qquad \sin\beta_1 \geqslant 0 \\ \cos\beta_2 &= -\left(\frac{m_2 m_3}{(m_1+m_2)(m_1+m_3)}\right)^{1/2}, \qquad \sin\beta_2 \leqslant 0 \\ \beta_3 &= 0. \end{aligned} \tag{11}$$

For three identical particles we have

$$\beta_1 = -\beta_2 = \frac{2\pi}{3}. \tag{12}$$

The transformation properties of the coordinates under permutations of the three particles become very simple. It is obvious from the definitions that r and ψ are invariants, while φ transforms as

$$\begin{aligned} E\varphi &= \varphi \\ P_{12}\varphi &= -\varphi \\ P_{23}\varphi &= -\varphi+\tfrac{4}{3}\pi \\ P_{13}\varphi &= -\varphi-\tfrac{4}{3}\pi \\ C\varphi &= \varphi+\tfrac{4}{3}\pi \\ C^2\varphi &= \varphi-\tfrac{4}{3}\pi. \end{aligned} \tag{13}$$

Here E denotes the identity element, P_{ij} a permutation of two particles and C the cyclic permutation. The Euler angles remain unaltered under E, C and C^2, while under exchanges of a pair they transform as

$$P_{ij}\begin{pmatrix}\alpha\\ \beta\\ \gamma\end{pmatrix} = \begin{pmatrix}\alpha\\ \beta-\pi\\ \pi-\gamma\end{pmatrix}. \tag{14}$$

With these new coordinates the Hamiltonian for three free particles becomes—in the centre of mass system—

$$H_0 = -\frac{1}{2\mu}\left[\frac{1}{r^5}\frac{\partial}{\partial r}\left(r^5\frac{r}{\partial r}\right)-\frac{\Lambda^2}{r^2}\right]. \tag{15}$$

Λ^2 is the operator of grand angular momentum, its eigenvalues are $K(K+4)$, where K is an integer, so $-\Lambda^2/r^2$ represents a generalized angular momentum barrier. The calculation of Λ^2 is straightforward:

$$\begin{aligned}\Lambda^2 = &-\frac{1}{\sin 4\psi}\frac{\partial}{\partial\psi}\left(\sin 4\psi\frac{\partial}{\partial\psi}\right)-\frac{4}{\cos^2 2\psi}\left(\frac{\partial^2}{\partial\varphi^2}+\frac{\partial^2}{\partial\gamma^2}\right)\\ &+\frac{4\sin 2\psi}{\cos^2 2\psi}\frac{\partial^2}{\partial\varphi\,\partial\gamma}+\frac{1}{\sin^2\psi}j_x^2+\frac{1}{\cos^2\psi}j_y^2+\frac{1}{\cos^2 2\psi}j_z^2.\end{aligned} \tag{16}$$

Here j_x, j_y and j_z are the angular momentum operators in the body-fixed coordinate system which coincide with the principal moments of inertia. The operator Λ^2 is the angular part of the six-dimensional Laplacian; it depends on five coordinates, its eigenfunctions are defined by

$$\Lambda^2 F^{K\nu JM\mu}(\alpha,\beta,\gamma;\varphi,\psi) = K(K+4)F^{K\nu JM\mu}(\alpha,\beta,\gamma;\varphi,\psi) \tag{17}$$

and can therefore be classified by five quantum numbers. They are simultaneous eigenfunctions of the following five operators:

(i) the grand angular momentum Λ^2, with eigenvalues $K(K+4)$ where $K = 0, 1, 2, \ldots$;

(ii) the operator $S = 2i\partial/\partial\varphi$ which is connected with permutations of the three particles and has eigenvalues $\nu = K, K-2, \ldots, -K+2, -K$;

(iii) the square of angular momentum $\boldsymbol{J}^2$, with eigenvalues $J(J+1)$ where $J \leqslant K$;

(iv) the space-fixed z component J_z of angular momentum with eigenvalues $M = -J, -J+1, \ldots, J-1, J$;

(v) an operator solving the degeneracy of the linearly independent solutions still existing for given values of K, v, J and M. The set of thus orthogonalized functions is distinguished by the quantum number μ in (17).

These properties suggest the expression of F as the finite sum ($|N| \leqslant J$)

$$F^{KvJM\mu}(\alpha, \beta, \gamma, \varphi, \psi) = \mathrm{e}^{-\mathrm{i}\frac{1}{2}v\varphi} \sum_N D^J_{MN}(\alpha, \beta, \gamma) g_N^{KvJ\mu}(\psi). \tag{18}$$

Putting (18) in (17) we obtain a system of coupled differential equations for the functions $g_N(\psi)$ belonging to each set of quantum numbers K, v, J, μ and independent of M in consequence of the Wigner–Eckart theorem:

$$\left[-\frac{1}{\sin 4\psi}\frac{\mathrm{d}}{\mathrm{d}\psi}\left(\sin 4\psi \frac{\mathrm{d}}{\mathrm{d}\psi}\right) - K(K+4) + \frac{v^2 + N^2 - 2vN \sin 2\psi}{\cos^2 2\psi} + 2\frac{J(J+1) - N^2}{\sin^2 2\psi}\right] g_N(\psi)$$

$$= -\frac{\cos 2\psi}{\sin^2 2\psi}(\langle JN|j_+^2|JN-2\rangle g_{N-2}(\psi) + \langle JN|j_-^2|JN+2\rangle g_{N+2}(\psi))$$

$$N = -J, \ldots, J. \tag{19}$$

We can state some general features of the system:

(i) in consequence of the Wigner–Eckart theorem the system is independent of M and we will therefore leave it out;

(ii) the $g_N^{KvJ\mu}$ for even and odd N are coupled separately and only one system has a non-trivial solution for given K, v and J;

(iii) it can easily be seen that

$$g_N^{K-vJ\mu}(\psi) = g_{-N}^{KvJ\mu}(\psi)$$

for $v \neq 0$, so that we have to solve (19) only for $v \geqslant 0$;

(iv) for $J \geqslant 2$ and given K, v and J there can be more than one independent solution of (19). For practical purposes one must orthogonalize these functions and they are then labelled by the quantum number μ.

Whitten and Smith (1968) have shown that a solution of (19) can be written in the form

$$g_N^{KvJ\mu}(\psi) = \sum_k^{K/2} \beta_{kN}^{KvJ\mu}\, d^k_{\frac{1}{2}v\frac{1}{2}N}(\tfrac{1}{2}\pi - 2\psi). \tag{20}$$

The system of linear equations holding for the coefficients β, however, turns out to be so cumbersome that its solution seems rather difficult, except in the simplest cases.

3. Solution of the differential equations

In order to solve the system (19) we therefore have chosen another decomposition of the functions g_N,

$$g_N^{KvJ\mu}(\psi) = (-1)^{(v-N)/2}(1+x)^{(v+N)/4}(1-x)^{(v-N)/4} \sum_{k=0}^{(K-v)/2} \alpha_k^N(K, v, J, \mu) x^k \tag{21}$$

with $x = \sin 2\psi$, ie $g_N(\psi)$ is equal to $\mathrm{d}^{\frac{1}{2}v}_{\frac{1}{2}v\frac{1}{2}N}(\frac{1}{2}\pi - 2\psi)$ times a polynomial in $\sin 2\psi$, which has the degree $(k - v)/2$. Therefore equation (21) is valid only for $v \geqslant J$. For N running from $-J$ to $+J$ there would occur for $v < J$ d-functions with lower indices greater than the upper index. Therefore one has to modify the *ansatz* (21) for $|N| > \nu$. If we choose for $N > \nu \geqslant 0$

$$g_N^{K\nu J\mu}(\psi) = (-1)^{(\nu-N)/2}(1+x)^{(N+\nu)/4}(1-x)^{(N-\nu)/4} \sum_{k=0}^{(K-N)/2} \alpha_k^N(K,\nu,J,\mu)x^k \tag{22}$$

and for $-N > \nu \geqslant 0$

$$g_N^{K\nu J\mu}(\psi) = (-1)^{(\nu-N)/2}(1+x)^{(|N|-\nu)/4}(1-x)^{(|N|+\nu)/4} \sum_{k=0}^{(K-|N|)/2} \alpha_k^N(K,\nu,J,\mu)x^k \tag{23}$$

with $x = \sin 2\psi$, the system of equations for the unknown coefficients α_k^N is very similar to that one for $\nu < J$ and is solved in the same way, perhaps with slight modifications.

Putting (21) in (19) we easily find a system of linear equations for the unknown coefficients α_k^N for every set K, ν, J, μ henceforward omitted:

$$\begin{aligned}\{k^2-\tfrac{1}{2}[J(J+1)-N^2]\}\alpha_k^N + D_+\alpha_k^{N-2} + D_-\alpha_k^{N+2} + [N(k-1)+\tfrac{1}{2}N]\alpha_{k-1}^N - D_+\alpha_{k-1}^{N-2} \\ + D_-\alpha_{k-1}^{N+2} + [(K+\nu)/2+k][(K-\nu)/2-k+2]\alpha_{k-2}^N = 0\end{aligned} \tag{24}$$

with $0 \leqslant k \leqslant (K-\nu)/2$,

$$N = \begin{cases} -J, -J+2, \ldots, J-2, J & \text{for } J+K \text{ even} \\ -J+1, -J+3, \ldots, J-3, J-1 & \text{for } J+K \text{ odd} \end{cases}$$

and

$$D_\pm = \tfrac{1}{4}\langle JN|j_\pm^2|JN\mp 2\rangle.$$

In the system (24) the number of non-trivial equations exceeds that of unknown coefficients by J for odd, and by $J+1$ for even $J+K$. We should therefore expect that no solution exists at all. We shall see, however, by closer inspection that even several solutions will exist for a given set of values K, ν, J distinguished by the superscript μ in (21).

In the following we confine ourselves to even values of $J+K$ (giving results for odd $J+K$ in the appendix). We then collect each set of α's for different N's in a vector

$$\boldsymbol{\alpha}_k^\dagger = (\alpha_k^{-J}, \alpha_k^{-J+2}, \ldots, \alpha_k^{J-2}, \alpha_k^J) \tag{25}$$

where $k = 0, 1, \ldots, (K-\nu)/2$. The system (3.2) thus can be written in matrix form,

$$A_k\boldsymbol{\alpha}_k + B_{k-1}\boldsymbol{\alpha}_{k-1} + C_{k-2}\boldsymbol{\alpha}_{k-2} = 0, \qquad k = 0, 1, \ldots, (K-\nu)/2. \tag{26}$$

A_k and B_k are tridiagonal matrices, the Nth row of A_k is

$$(0, \ldots, 0, \tfrac{1}{4}\langle JN|j_+^2|JN-2\rangle, k^2-\tfrac{1}{2}[J(J+1)-N^2], \tfrac{1}{4}\langle JN|j_-^2|JN+2\rangle, 0, \ldots, 0), \tag{27}$$

the same row of B_k is

$$(0, \ldots, 0, -\tfrac{1}{4}\langle JN|j_+^2|JN-2\rangle, (k+\tfrac{1}{2})N, \tfrac{1}{4}\langle JN|j_-^2|JN+2\rangle, 0, \ldots, 0). \tag{28}$$

C_k is the $(J+1)$-dimensional unit matrix multiplied by $[(K+\nu)/2+2+k][(K-\nu)/2-k]$. The key to the solution of (26) is the following.

Theorem 1

(i) The symmetric matrices $A_k, k = 0, 1, \ldots, J$ have eigenvectors $\boldsymbol{a}_k$ to the eigenvalue zero, ie

$$A_k\boldsymbol{a}_k = 0, \qquad k = 0, 1, \ldots, J. \tag{29}$$

(ii) These vectors $\boldsymbol{a}_k$ form an orthogonal basis in the space of $(J+1)$-dimensional vectors, ie

$$(\boldsymbol{a}_n, \boldsymbol{a}_m) = 0 \qquad n \neq m,$$

and each $\boldsymbol{\alpha}_k$ is a linear combination of the $\boldsymbol{a}_k$.

The rather complicated proof of the existence of the eigenvectors $\boldsymbol{a}_k$ will be omitted. It has, however, been given rigorously (Mayer 1974). That the vectors $\boldsymbol{a}_k$ form a basis is easily seen, since from (27) there follows

$$A_k = 1k^2 + A_0 \tag{30}$$

and therefore

$$A_0\boldsymbol{a}_k = -k^2\boldsymbol{a}_k, \qquad k = 0, 1, \ldots, J. \tag{31}$$

Since A_0 is a real symmetric matrix, its $J+1$ eigenvectors $\boldsymbol{a}_k$ must form an orthogonal set.

The $\boldsymbol{a}_k$ can be expressed in terms of $\boldsymbol{a}_0$ which has the components

$$a_0^N = \frac{1}{2^J}\left[\binom{J+N}{(J+N)/2}\binom{J-N}{(J-N)/2}\right]^{1/2}.$$

We then have

$$\begin{aligned} \boldsymbol{a}_1 &= N\boldsymbol{a}_0 \\ \boldsymbol{a}_2 &= [-\tfrac{1}{2}J(J+1)+N^2]\boldsymbol{a}_0 \\ \boldsymbol{a}_{k+1} &= N\boldsymbol{a}_k - \tfrac{1}{4}[J(J+1)-k(k-1)]\boldsymbol{a}_{k-1}, \qquad 2 \leqslant k \leqslant J-1. \end{aligned} \tag{32}$$

Here N is the diagonal matrix with the elements

$$-J, \; -J+2, \ldots, J-2, J.$$

Application of the B matrices (3.6) yields the relations

$$\begin{aligned} B_0\boldsymbol{a}_0 &= 0 \\ B_1\boldsymbol{a}_1 &= J(J+1)\boldsymbol{a}_0 \\ B_k\boldsymbol{a}_k &= \tfrac{1}{2}k[J(J+1)-k(k-1)]\boldsymbol{a}_{k-1}, \qquad 2 \leqslant k \leqslant J \end{aligned} \tag{33}$$

and

$$\begin{aligned} B_l\boldsymbol{a}_0 &= l\boldsymbol{a}_0 \\ B_l\boldsymbol{a}_1 &= (l-1)\boldsymbol{a}_2 + \tfrac{1}{2}(l+1)J(J+1)\boldsymbol{a}_0 \\ B_l\boldsymbol{a}_k &= (l-k)\boldsymbol{a}_{k+1} + \tfrac{1}{4}(l+k)[J(J+1)-k(k-1)]\boldsymbol{a}_{k-1}, \qquad 2 \leqslant k \leqslant J \\ l &= 0, 1, 2, \ldots. \end{aligned} \tag{34}$$

Knowing the basis vectors $\boldsymbol{a}_k$ and $A_l\boldsymbol{a}_k$, $B_l\boldsymbol{a}_k$, we can expand the solution vectors $\boldsymbol{\alpha}_k$ into linear combinations of the $\boldsymbol{a}_k$:

$$\boldsymbol{\alpha}_k = \sum_{\rho=0}^{J} \sigma_\rho^k \boldsymbol{a}_\rho. \tag{35}$$

The first equation of the system (26) is

$$A_0\boldsymbol{\alpha}_0 = 0, \tag{36}$$

hence from (31), $\boldsymbol{\alpha}_0 = \sigma_0^0 \boldsymbol{a}_0$ so that σ_0^0 is not determined by this equation. Since $B_0 \boldsymbol{a}_0 = 0$ we have from (26)

$$A_1 \boldsymbol{\alpha}_1 + B_0 \boldsymbol{\alpha}_0 = 0. \tag{37}$$

There follows $A_1 \boldsymbol{\alpha}_1 = 0$ or, from (35),

$$\sum_{\rho=0}^{J} \sigma_0^1 A_1 \boldsymbol{a}_\rho = 0.$$

From (30) we have, on the other hand,

$$A_1 \boldsymbol{a}_\rho = (1-\rho^2) \boldsymbol{a}_\rho$$

which for $\rho = 1$ vanishes. Hence the coefficient σ_1^1 cannot yet be determined.

It is easily seen by induction that the following theorem holds here.

Theorem 2

The vector $\boldsymbol{\alpha}_k, 0 \leqslant k \leqslant (K-v)/2$ is

$$\begin{aligned} &\text{(i)} \qquad \boldsymbol{\alpha}_k = \sum_{\rho=0}^{M_k} \sigma_{2\rho}^k \boldsymbol{a}_{2\rho} \qquad k \text{ even} \\ &\text{(ii)} \qquad \boldsymbol{\alpha}_k = \sum_{\rho=0}^{M_k} \sigma_{2\rho+1}^k \boldsymbol{a}_{2\rho+1} \qquad k \text{ odd} \end{aligned} \tag{38}$$

with $M_k = \min\{[k/2], [J/2]\}$, where the symbol $[x]$ means the largest integer less than or equal to x.

As $A_k \boldsymbol{a}_k = 0$ and $B_{k-1} \boldsymbol{a}_{k-1} \propto \boldsymbol{a}_{k-2}$, we have with (34) that the equation

$$A_k \boldsymbol{\alpha}_k + B_{k-1} \boldsymbol{\alpha}_{k-1} + C_{k-2} \boldsymbol{\alpha}_{k-2} = 0, \qquad k = 0, 1, \ldots, J$$

does not determine the coefficient σ_k^k of $\boldsymbol{\alpha}_k$. The unknown coefficients are now the σ_ρ^k. For these coefficients we get a system of linear equations by putting (38) into (26) and using the properties (32–34), where the number of equations is now less than the number of coefficients. The difference $N_J(K, v)$ between the number of unknown coefficients and the number of equations determining the σ_ρ^k depends on K and J:

$$N_J(K, v) = [P(K-J+2)/2] - [P((K-v)/2-J+1)/2] - [P((K+v)/2-J+1)/2] \tag{39}$$

with $P(x) = \frac{1}{2}(x+|x|)$ and $[x]$ as in theorem 2. We shall not give here in detail the system of linear equations for the σ_ρ^k: this can easily be done. But we must keep in mind that $N_J(K, v)$ is the number of linearly independent solutions of (2.8), and we will get these different solutions in a very natural manner by solving the system of linear equations for the σ_ρ^k. We still remark that (39) is in accordance with the result of Racah (1949), who has studied how many times an irreducible representation $D(J)$ of SO(3) appears in the decomposition of an irreducible representation (λ_1, λ_2) of SU(3).

4. Parity and symmetry properties of the hyperspherical functions

A reflection of the position vectors of three particles in the centre of mass system does not change the internal coordinates r, ψ, φ and the two Euler angles α, β, but the third Euler angle γ goes over into $\gamma + \pi$, and therefore in a γ-dependent D-function

$$D_{MN}^J(\alpha, \beta, \gamma+\pi) = (-1)^N D_{MN}^J(\alpha, \beta, \gamma). \tag{40}$$

Since $(-1)^N$ is always equal to $(-1)^K$, (equation (24)), the parity of the hyperspherical functions $F^{K\nu JM\mu}$ is $(-1)^K$.

If we interchange the identical particles 1 and 2 then φ is changed to $-\varphi$ and the three Euler angles transform as in equation (14). The coordinates r and ψ remain unaltered. From the definition of the $F^{K\nu JM\mu}$ in (18) and the transformation properties of D-functions we have

$$P_{12}F^{K\nu JM\mu} = (-1)^J F^{K\nu JM\mu}. \tag{41}$$

Thus by defining

$$F_{\pm}^{K|\nu|JM\mu} = F^{K|\nu|JM\mu} \pm F^{K-|\nu|JM\mu}$$

we get eigenfunctions of P_{12} which are symmetric $(+)$ or antisymmetric $(-)$ for even J and vice versa for odd J:

$$P_{12}\begin{pmatrix} F_{+}^{K|\nu|JM\mu} \\ F_{-}^{K|\nu|JM\mu} \end{pmatrix} = (-1)^J \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} F_{+}^{K|\nu|JM\mu} \\ F_{-}^{K|\nu|JM\mu} \end{pmatrix}. \tag{42}$$

For three equal particles one has to take into account (13) and (14). Since we have already studied the transformation properties under P_{12} it is sufficient to do the same for the cyclic permutation C; all other group elements can be obtained by multiplication. The result for the F_+ and F_- is:

$$C\begin{pmatrix} F_{+}^{K|\nu|JM\mu} \\ F_{-}^{K|\nu|JM\mu} \end{pmatrix} = \begin{pmatrix} \cos\frac{2}{3}\pi|\nu| & -\mathrm{i}\sin\frac{2}{3}\pi|\nu| \\ -\mathrm{i}\sin\frac{2}{3}\pi|\nu| & \cos\frac{2}{3}\pi|\nu| \end{pmatrix} \begin{pmatrix} F_{+}^{K|\nu|JM\mu} \\ F_{-}^{K|\nu|JM\mu} \end{pmatrix}. \tag{43}$$

The characteristic angle $\frac{2}{3}\pi$ makes it necessary to distinguish between the several possible values of ν. For $|\nu| = 3n, n = 0, 1, 2, \ldots$, C becomes the identity matrix and F_+ and F_- are transformed separately corresponding to the two different one-dimensional irreducible representations of S_3, the group of permutations of three particles. For $|\nu| = 3n+1$, we have

$$C = \begin{pmatrix} -\frac{1}{2} & -\frac{1}{2}\mathrm{i}\sqrt{3} \\ -\frac{1}{2}\mathrm{i}\sqrt{3} & -\frac{1}{2} \end{pmatrix} \tag{44}$$

and therefore we get a two-dimensional irreducible representation of S_3. For $|\nu| = 3n+2$,

$$C = \begin{pmatrix} -\frac{1}{2} & \frac{1}{2}\mathrm{i}\sqrt{3} \\ \frac{1}{2}\mathrm{i}\sqrt{3} & -\frac{1}{2} \end{pmatrix}. \tag{45}$$

C belongs to another two-dimensional representation of S_3, which is equivalent to that one obtained for $|\nu| = 3n+1$. We thus have obtained functions $F_{\pm}^{K|\nu|JM\mu}$, which are simultaneously eigenfunctions of the total angular momentum J and its projection J_z and the group of transformations of three particles. Thus for problems with identical particles functions are available with defined behaviour with respect to exchange of identical particles.

In this work we have studied the solutions of the angular part of the Hamiltonian for three free particles. In general the potential between three particles will depend on all three internal variables r, ψ, φ but never on the Euler angles α, β, γ. The solution Ψ of the Schrödinger equation

$$(H_0 + V(r, \varphi, \psi))\Psi = E\Psi \tag{46}$$

can therefore be expanded into a series of hyperspherical functions for given J and M:

$$\Psi = \sum_{K\nu\mu} G_{K\nu\mu}(r) F_{\pm}^{K|\nu|JM\mu}. \tag{47}$$

For the functions $G_{K\nu\mu}(r)$ one obtains a system of differential equations

$$\left[\frac{\hbar^2}{2\mu}\left(\frac{\mathrm{d}^2}{\mathrm{d}r^2}+\frac{5}{r}\frac{\mathrm{d}}{\mathrm{d}r}-\frac{K(K+4)}{r^2}\right)+E\right]G_{K\nu\mu}(r) = \sum_{K'\nu'\mu'} \langle K\nu\mu|V|K'\nu'\mu'\rangle G_{K'\nu'\mu'}(r). \tag{48}$$

Calculations have been performed using equation (48) by several authors (Zickendraht 1965, Simonov and Badalyan 1967, Tartakovskii and Kozlovskii 1973) for total angular momentum $J = 0$. Using the results of this work one can perform calculations for arbitrary J.

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Appendix

A.1. Method of solution for $J+K$ odd

For $J+K$ odd, ie $N = -J+1, -J+3, \ldots J-3, J-1$, we define in analogy with (25) J-dimensional vectors

$$\boldsymbol{\alpha}_k^{\dagger} = (\alpha_k^{-J+1}, \alpha_k^{-J+3}, \ldots, \alpha_k^{J-3}, \alpha_k^{J-1}), \qquad k = 0, 1, \ldots, (K-\nu)/2. \tag{A.1}$$

The system (24) takes the same form as (26), the only difference being that the matrices and vectors are J-dimensional. The analogue of theorem 1 is the following theorem.

Theorem 3

(i) The symmetric matrices $A_k, k = 1, 2, \ldots, J$ have eigenvectors $\boldsymbol{a}_k$ to the eigenvalue zero, ie

$$A_k \boldsymbol{a}_k = 0, \qquad k = 1, 2, \ldots, J. \tag{A.2}$$

(ii) The vectors $\boldsymbol{a}_k, k = 1, \ldots, J$ form an orthogonal basis in the space of J-dimensional vectors.

The eigenvectors $\boldsymbol{a}_k$ have the following properties ($\boldsymbol{a}_0 \equiv 0!$):

(*a*)
$$\begin{aligned}
a_1^N &= 2^J\left[\binom{J+N}{(J+N)/2}\binom{J-N}{(J-N)/2}\right]^{1/2} \\
\boldsymbol{a}_2 &= N\boldsymbol{a}_1 \\
\boldsymbol{a}_{k+1} &= N\boldsymbol{a}_k - \tfrac{1}{4}[J(J+1)-k(k-1)]\boldsymbol{a}_{k-1}, \qquad 2 \leqslant k \leqslant J-1 \\
A_l\boldsymbol{a}_k &= (l^2-k^2)\boldsymbol{a}_k, \qquad 1 \leqslant k \leqslant J, \qquad l = 0, 1, 2, \ldots .
\end{aligned} \tag{A.3}$$

$$(b) \qquad \begin{aligned} B_1 \boldsymbol{a}_1 &= 0 \\ B_k \boldsymbol{a}_k &= \tfrac{1}{2}k[J(J+1)-k(k-1)]\boldsymbol{a}_{k-1}, \qquad 2 \leqslant k \leqslant J \end{aligned} \tag{A.4}$$

$$(c) \qquad \begin{aligned} B_l \boldsymbol{a}_1 &= (l-1)\boldsymbol{a}_2 \\ B_l \boldsymbol{a}_k &= (l-k)\boldsymbol{a}_{k+1} + \tfrac{1}{4}(l+k)[J(J+1)-k(k-1)]\, \boldsymbol{a}_{k-1} \\ & \qquad 2 \leqslant k \leqslant J, \qquad l = 0, 1, 2, \ldots . \end{aligned} \tag{A.5}$$

With these vectors the method of solving (24) is quite the same as in the case $J+K$ even. The relation (39) still holds for this case.

A.2. *Solution for* $J = 0, 1, 2$

According to the *ansatz* (21),

$$F^{K\nu JM\mu}(\alpha, \beta, \gamma, \varphi, \psi) = \mathrm{e}^{-\mathrm{i}\frac{1}{2}\nu\varphi} \sum_N D^J_{MN}(\alpha, \beta, \gamma) g_N^{K\nu J\mu}(\psi) \tag{A.6}$$

we give here the solutions $g_N^{K\nu J\mu}(\psi)$ for $\nu \geqslant 0$. In this section we put $x = \sin 2\psi$. $P_n^{(\alpha,\beta)}$ are the well known Jacobi polynomials with the normalization $P_n^{(\alpha,\beta)}(1) = \binom{n+\alpha}{n}$ as given in Erdélyi *et al* (1953).

A.2.1. $J = 0$

This case is well known. (Simonov 1966, Zickendraht 1965.)

$$g_0^{K\nu 0}(\psi) = d^{\frac{1}{4}K}_{\frac{1}{4}\nu\frac{1}{4}\nu}(4\psi) \tag{A.7}$$

and therefore $K = 0, 2, 4, 6, \ldots, \nu = -K, -K+4, \ldots, K-4, K$.

A.2.2. $J = 1$

(i) K even, therefore ν even and $N = 0$

$$g_0^{K\nu 1}(\psi) = d^{\frac{1}{4}K}_{\frac{1}{4}(\nu+2)\frac{1}{4}(\nu-2)}(4\psi) \tag{A.8}$$

$K = 2, 4, 6, \ldots, \nu = -K+2, -K+6, \ldots, K-6, K-2$.
(ii) K odd. Here we determine, according to (32), the basis vectors $\boldsymbol{a}_0$ and $\boldsymbol{a}_1$:

$$\boldsymbol{a}_0 = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix} \qquad \boldsymbol{a}_1 = \frac{1}{\sqrt{2}}\begin{pmatrix} -1 \\ 1 \end{pmatrix}. \tag{A.9}$$

The solutions g are

(*a*) $(K-\nu)/2$ even

$$\begin{aligned} g_N^{K\nu 1}(\psi) = (-1)^{(\nu-N)/2}(1+x)^{(\nu+N)/4}(1-x)^{(\nu-N)/4}\big[&a_0^N P^{(0,(\nu+1)/2)}_{(K-\nu)/4}(1-2x^2) \\ &+ a_1^N x P^{(1,(\nu+1)/2)}_{(K-\nu)/4-1}(1-2x^2)\big]. \end{aligned} \tag{A.10}$$

(*b*) $(K-\nu)/2$ odd

$$\begin{aligned} g_N^{K\nu 1}(\psi) = (-1)^{(\nu-N)/2}(1+x)^{(\nu+N)/4}(1-x)^{(\nu-N)/4}\{&a_0^N P^{(0,(\nu+1)/2)}_{(K-\nu-2)/4}(1-2x^2) \\ &- a_1^N x[(K+\nu+4)/(K-\nu+2)] P^{(1,(\nu+1)/2)}_{(K-\nu-2)/4}(1-2x^2)\}. \end{aligned} \tag{A.11}$$

A.2.3. $J = 2$

(i) K odd, ν odd, $N = \pm 1$

Here we need the basis vectors $\boldsymbol{a}_1$ and $\boldsymbol{a}_2$, according to (A.3):

$$\boldsymbol{a}_1 = \left(\frac{3}{2}\right)^{1/2}\begin{pmatrix}1\\1\end{pmatrix} \qquad \boldsymbol{a}_2 = \left(\frac{3}{2}\right)^{1/2}\begin{pmatrix}-1\\1\end{pmatrix}.$$

(*a*) $(K-\nu)/2$ even

$$g_N^{K\nu 2}(\psi) = (-1)^{(\nu-N)/2}(1+x)^{(\nu+N)/4}(1-x)^{(\nu+N)/4} \times \left(a_1^N \frac{x}{(K-\nu)/4} P^{(1,(\nu+1)/2)}_{(K-\nu)/4-1}(1-2x^2) - a_2^N \frac{x^2(K+\nu+6)}{\frac{1}{4}(K-\nu)(K-\nu+4)} \times P^{(2,(\nu+1)/2)}_{(K-\nu)/4-1}(1-2x^2)\right). \tag{A.12}$$

(*b*) $(K-\nu)/2$ odd

$$g_N^{K\nu 2}(\psi) = (-1)^{(\nu-N)/2}(1+x)^{(\nu+N)/4}(1-x)^{(\nu-N)/4} \times \left(a_1^N \frac{x}{(K-\nu+2)/4} P^{(1,(\nu+1)/2)}_{(K-\nu-2)/4}(1-2x^2) + a_2^N \frac{x^2}{(K-\nu+2)/4} \times P^{(2,(\nu+1)/2)}_{(K-\nu-2)/4}(1-2x^2)\right). \tag{A.13}$$

(ii) K even, ν even, $N = -2, 0, 2$

The basis vectors $\boldsymbol{a}_0$, $\boldsymbol{a}_1$, $\boldsymbol{a}_2$ are:

$$\boldsymbol{a}_0 = \tfrac{1}{2}\begin{pmatrix}\sqrt{\frac{3}{2}}\\ 1\\ \sqrt{\frac{3}{2}}\end{pmatrix} \qquad \boldsymbol{a}_1 = \begin{pmatrix}-\sqrt{\frac{3}{2}}\\ 0\\ \sqrt{\frac{3}{2}}\end{pmatrix} \qquad \boldsymbol{a}_2 = \tfrac{1}{2}\begin{pmatrix}\sqrt{\frac{3}{2}}\\ -3\\ \sqrt{\frac{3}{2}}\end{pmatrix}.$$

Now we must distinguish between the cases $\nu = 0$, ie $\nu < J$, and $\nu \geqslant 2$, ie $\nu \geqslant J$.

(*a*) $\nu = 0$

(1) $K/2$ odd

$$g_N^{K02}(\psi) = (-1)^{N/2}(1-x^2)^{N/4}\left(a_0^N P^{(0,1)}_{(K-2)/4}(1-2x^2) - a_2^N \frac{x^2}{3}\frac{K+6}{K+2} \times P^{(2,1)}_{(K-2)/4-1}(1-2x^2)\right). \tag{A.14}$$

(2) $K/2$ even (two linearly independent solutions)

$$g_N^{K021}(\psi) = (-1)^{N/2}(1-x^2)^{N/4} a_1^N x \frac{K+4}{K} P^{(1,1)}_{(K/4)-1}(1-2x^2) \tag{A.15}$$

$$g_N^{K022}(\psi) = (-1)^{N/2}(1-x^2)^{N/4}\left[a_0^N\left(P^{(0,0)}_{K/4}(1-2x^2) + \frac{3}{K}x^2 P^{(1,1)}_{(K/4)-1}(1-2x^2)\right) + a_2^N x^2 \frac{1}{(K/4)(K/4+1)}\{[(K/4)(K/4+1)+\tfrac{1}{2}]P^{(2,0)}_{(K/4)-1}(1-2x^2) - \tfrac{1}{4}(K/4+2)x^2 P^{(3,1)}_{(K/4)-2}(1-2x^2)\}\right]. \tag{A.16}$$

(*b*) $\nu \geqslant 2$

(1) $(K-\nu)/2$ odd

$$g_N^{K\nu 2}(\psi) = (-1)^{(\nu-N)/2}(1+x)^{(\nu+N)/4}(1-x)^{(\nu-N)/4}\Bigg[a_0^N P^{(0,\nu/2+1)}_{(K-\nu-2)/4}(1-2x^2)$$

$$-a_1^N\frac{x}{6}\left(\frac{4(\nu+3)}{K-\nu+2}P^{(1,\nu/2)}_{(K-\nu-2)/4}(1-2x^2)-4x^2\frac{K+\nu+6}{K-\nu+2}P^{(2,\nu/2+1)}_{(K-\nu-2)/4-1}(1-2x^2)\right)$$

$$-a_2^N\frac{x^2}{3}\,\frac{K+\nu+6}{K-\nu+2}P^{(2,\nu/2+1)}_{(K-\nu-2)/4-1}(1-2x^2)\Bigg]. \qquad \text{(A.17)}$$

(2) $(K-\nu)/2$ even (two linearly independent solutions)

$$g_N^{K\nu 21}(\psi) = (-1)^{(\nu-N)/2}(1+x)^{(\nu+N)/4}(1-x)^{(\nu-N)/4}$$

$$\times\left(a_0^N P^{(0,\nu/2)}_{(K-\nu)/4}(1-2x^2)+a_2^N x^2\frac{K+\nu+4}{K-\nu+4}P^{(2,\nu/2)}_{(K-\nu)/4-1}(1-2x^2)\right) \qquad \text{(A.18)}$$

$$g_N^{K\nu 22}(\psi) = (-1)^{(\nu-N)/2}(1+x)^{(\nu+N)/4}(1-x)^{(\nu-N)/4}$$

$$\times\Bigg[a_0^N P^{(0,\nu/2+1)}_{(K-\nu)/4}(1-2x^2)+a_1^N\tfrac{2}{3}xP^{(1,\nu/2+1)}_{(K-\nu)/4-1}(1-2x^2)$$

$$+a_2^N\frac{x^2}{6}\Bigg(4\frac{K+(K-\nu)/2+2}{K-\nu+4}P^{(2,\nu/2)}_{(K-\nu)/4-1}(1-2x^2)+2x^2\frac{K+\nu+8}{K-\nu+4}$$

$$\times P^{(3,\nu/2+1)}_{(K-\nu)/4-2}(1-2x^2)\Bigg)\Bigg]. \qquad \text{(A.19)}$$

References

Dragt A J 1965 *J. Math. Phys.* **6** 533

Erdélyi A, Magnus W, Oberhettinger F and Tricomi F G 1953 *Higher Transcendental Functions* vol 2 (New York: McGraw-Hill)

Mayer H 1974 *PhD Thesis* University of Freiburg

Racah G 1949 *Rev. Mod. Phys.* **21** 494

Rose E 1967 *Elementary Theory of Angular Momentum* (New York: Wiley)

Simonov Y A 1966 *Jadern. Fiz.* **3** 630 (1966 *Sov. J. Nucl. Phys.* **3** 461)

Simonov Y A and Badalyan A M 1967 *Jadern. Fiz.* **5** 88 (1967 *Sov. J. Nucl. Phys.* **5** 60)

Smith F T 1960 *Phys. Rev.* **120** 1058

Tartakovskii V K and Kozlovskii I V 1973 *Jadern. Fiz.* **17** 278 (1973 *Sov. J. Nucl. Phys.* **17** 142)

Whitten R C and Smith F T 1968 *J. Math. Phys.* **9** 1103

Zickendraht W 1965 *Ann. Phys., NY* **35** 18