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Special case of the separation of variables in the multidimensional Schrödinger equation

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Abstract. We obtain a wide class of multidimensional polynomial potentials for which the Schrödinger equation allows the separation of variables in generalised ellipsoidal coordinates.

It is well known that multidimensional quantum mechanical models with polynomial potentials play an important role in many fields of quantum physics. The study of the spectra of such models becomes essentially simple when the separation of variables in the Schrödinger equation is permissible. As an example, we refer to the well known cases of the spherical- and cylindrical-symmetric potentials.

In addition to spherical and cylindrical coordinates, ellipsoidal ones are very useful for solving certain equations of mathematical physics. For example, in Mardoyan *et al* (1985) the multidimensional harmonic oscillator in ellipsoidal coordinates has been studied in detail. Unfortunately, until recently these coordinates had not been considered in connection with quantum mechanical problems with polynomial anharmonicity. The first step in this direction was made, apparently, in the work of Turbiner and Ushveridze (1986), where the most general form of two-dimensional polynomial potentials allowing the separation of variables in ellipsoidal and parabolic coordinates was presented.

In the present paper, which is quite independent of the above-mentioned work, we consider the multidimensional case. We show that there exists a wide class of multidimensional polynomial potentials without any spherical or cylindrical symmetry, for which the Schrödinger equation

$$\left(-\sum_{i=1}^{N}\frac{\partial^2}{\partial x_i^2}+V-E\right)\psi=0 \tag{1}$$

can be reduced to the system of one-dimensional spectral equations by means of separation of variables in generalised ellipsoidal coordinates. The three-dimensional case of these coordinates is described in Korn and Korn (1961).

The connection between the cartesian, $\{x_i\}$, and the generalised (multidimensional) ellipsoidal coordinates, which we denote by $\{\lambda_i\}$, can be expressed as follows:

$$x_i^2=\prod_{k=1}^{N}(\lambda_k-a_i)\left(\prod_{k=1,k\neq i}^{N}(a_k-a_i)\right)^{-1}. \tag{2}$$

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Here a_i are constants determining the intervals in which the λ_i coordinates change,

$$a_1 < \lambda_1 < a_2 < \lambda_2 < \ldots < a_N < \lambda_N < \infty. \tag{3}$$

In the new variables the Schrödinger equation (1) assumes the form

$$\left(- \sum_{i=1}^{N} \frac{4(Q(\lambda_i))^{1/2}}{\prod_{k=1,k\neq i}^{N} (\lambda_i - \lambda_k)} \frac{\partial}{\partial \lambda_i} [(Q(\lambda_i))^{1/2} \partial / \partial \lambda_i] + V - E \right) \psi = 0 \tag{4}$$

where

$$Q(\lambda) = \prod_{k=1}^{N} (\lambda - a_k). \tag{5}$$

In order to investigate the possibility of separation of variables in equation (4), let us introduce the special function

$$f_L^{(N)}(\lambda) \equiv \sum_{k=1}^{N} \lambda_k^{N-1+L} \left(\prod_{i=1,i\neq k}^{N} (\lambda_k - \lambda_i) \right)^{-1} \tag{6}$$

invariant under all transformations of the permutation group.

Statement 1. If $-(N-1) \leqslant L < 0$, then the function $f_L^{(N)}(\lambda)$ is identically zero, and if $L \geqslant 0$, $f_L^{(N)}(\lambda)$ is the Lth-order polynomial of the form

$$f_L^{(N)}(\lambda) = \sum_{1 l_1 + \ldots + L l_L = L} f_{l_1 \ldots l_L} \sigma_1^{l_1}(\lambda) \ldots \sigma_L^{l_L}(\lambda). \tag{7}$$

Here $f_{l_1 \ldots l_L}$ are constants and

$$\sigma_i(\lambda) = \begin{cases} \sum_{k_1 < \ldots < k_i} \lambda_{k_1} \cdot \ldots \cdot \lambda_{k_i} & 1 \leqslant i \leqslant N \\ 1 & i = 0 \\ 0 & i > N \end{cases} \tag{8}$$

are the elementary symmetric polynomials.

Proof. Let I and J be arbitrary fixed numbers, $I \neq J$. Introducing the function

$$U_{IJ}(\lambda) \equiv \lambda^{N-1+L} \left(\prod_{i=1,i\neq I,i\neq J}^{N} (\lambda - \lambda_i) \right)^{-1} \tag{9}$$

we can rewrite formula (6) in the following form:

$$f_L^{(N)}(\lambda) = \frac{U_{IJ}(\lambda_I) - U_{IJ}(\lambda_J)}{\lambda_I - \lambda_J} + \sum_{\substack{k=1 \\ k\neq I, k\neq J}}^{N} \lambda_k^{N-1+L} \left(\prod_{i=1,i\neq k}^{N} (\lambda_k - \lambda_i) \right)^{-1} \tag{10}$$

From the representation (10) it follows that the function $f_L^{(N)}(\lambda)$ remains finite if λ_I tends to λ_J. The fact that the finiteness of $f_L^{(N)}(\lambda)$ is fulfilled for any I and J implies that this function is regular everywhere.

On the other hand, from the definition (6) it follows that the function $f_L^{(N)}(\lambda)$ can be represented as a fraction whose numerator is a homogeneous polynomial of $[N(N-1)+L]$th order. The denominator of this fraction is also a homogeneous polynomial of $[N(N-1)]$th order and has the form $\prod_{i<k} (\lambda_i - \lambda_k)^2$. We can see that it vanishes if $\lambda_i = \lambda_k$. The fact that the function $f_L^{(N)}(\lambda) = 0$ has no poles means that the numerator in the fraction can be divided by the denominator without remainder. Hence $f_L^{(N)}(\lambda) = 0$ if $-(N-1) \leqslant L < 0$, and $f_L^{(N)}(\lambda)$ is the Lth-order polynomial when $L \geqslant 0$. Since $f_L^{(N)}(\lambda)$ is invariant under all transformations of the permutation group, it can be expressed via the elementary symmetric polynomials defined by (8). Thus statement 1 is proved.

It is not difficult to calculate several first functions $f_L^{(N)}(\lambda)$. They are

$$\begin{aligned} f_0^{(N)}(\lambda) &= 1 \\ f_1^{(N)}(\lambda) &= \sigma_1(\lambda) \\ f_2^{(N)}(\lambda) &= \sigma_1^2(\lambda) - \sigma_2(\lambda) \\ f_3^{(N)}(\lambda) &= \sigma_1^3(\lambda) - 2\sigma_1(\lambda)\sigma_2(\lambda) + \sigma_3(\lambda). \end{aligned} \tag{11}$$

Statement 2. If the potential V in the λ coordinates has the form

$$V = \sum_{k=1}^{N} \lambda_k^{N-1} P_L(\lambda_k)\left(\prod_{i\neq k} (\lambda_k - \lambda_i)\right)^{-1} \qquad P_L(\lambda) = \sum_{l=0}^{L} P_{L,l}\lambda^l \tag{12}$$

then in the initial x coordinates it is a polynomial.

Proof. From definition (2) it follows that

$$\sum_{n=1}^{N} (-1)^n a_i^n \sigma_n(\lambda) = x_i^2 \prod_{k\neq i}^{N} (a_k - a_i). \tag{13}$$

These relations can be considered as the linear equations for $\sigma_n(\lambda)$. Solving system (13) we obtain

$$\sigma_n(\lambda) = \sigma_n(a) + \sum_k \sigma_{n-1}^{(k)}(a) x_k^2 \tag{14}$$

where $\sigma_n^{(k)}(a)$ are defined as the nth-order symmetric polynomials of $a_1, a_2, \ldots, a_{k-1}, a_{k+1}, \ldots, a_N$. According to statement 1 the potential V depends polynomially on $\sigma_n(\lambda)$, and, hence, it is the Lth-order polynomial of x_k^2. The statement is proved.

For several values of n in (14) we obtain

(i) $N=2$

$$\begin{aligned} \sigma_1(\lambda) &= (x_1^2 + x_2^2) + (a_1 + a_2) \\ \sigma_2(\lambda) &= (a_2 x_1^2 + a_1 x_2^2) + a_1 a_2 \end{aligned} \tag{15}$$

(ii) $N=3$

$$\begin{aligned} \sigma_1(\lambda) &= (x_1^2 + x_2^2 + x_3^2) + (a_1 + a_2 + a_3) \\ \sigma_2(\lambda) &= (a_1 + a_2 + a_3)(x_1^2 + x_2^2 + x_3^2) - (a_1 x_1^2 + a_2 x_2^2 + a_3 x_3^2) + (a_1 a_2 + a_1 a_3 + a_2 a_3) \\ \sigma_3(\lambda) &= (a_2 a_3 x_1^2 + a_1 a_3 x_2^2 + a_1 a_2 x_3^2) + a_1 a_2 a_3. \end{aligned} \tag{16}$$

Statement 3. If the potential V in λ coordinates has the form (12), the Schrödinger equation (4) allows the separation of variables.

Proof. According to statement 1, the constant E can be represented in the form

$$E \equiv \sum_k \left(E\lambda_k^{N-1} + \sum_{n=0}^{N-2} \Gamma_n \lambda_k^n\right)\left(\prod_{i\neq k}^{N} (\lambda_k - \lambda_i)\right)^{-1}. \tag{17}$$

Substituting (17) and (12) into (4) and taking

$$\psi = \psi_1(\lambda_1) \ldots \psi_N(\lambda_N) \tag{18}$$

one obtains the system of one-dimensional spectral equations

$$\left(-Q(\lambda_k)\frac{\partial^2}{\partial\lambda_k^2}-\tfrac{1}{2}Q'(\lambda_k)\frac{\partial}{\partial\lambda_k}+P_L(\lambda_k)\right)\psi_k(\lambda_k)$$

$$=\left(E\lambda_k^{N-1}+\sum_{n=0}^{N-2}\Gamma_n\lambda_k^n\right)\psi_k(\lambda_k) \qquad k=1,\ldots,N. \tag{19}$$

Here the energy E is the spectral parameter of the initial problem, and Γ_n are the separation constants playing the role of the auxiliary spectral parameters of system (19). Thus the statement is proved.

Letting

$$P_L(\lambda)=\sum_{l=0}^{L}P_{L,l}\lambda^l \tag{20}$$

and using (6), (7) and (12) we get

$$V=\sum_{l=0}^{L}P_{L,l}f_l(\lambda). \tag{21}$$

Substituting (15) and (16) into (11) and (21) we obtain the explicit form of the potentials in x representation, allowing the separation of variables in generalised ellipsoidal coordinates.

Now let us consider concrete examples of potentials for which the separtion of variables in λ coordinates is permissible.

(i) Two-dimensional quartic anharmonic oscillator, $N=2$, $L=2$:

$$V\sim(x_1^2+x_2^2)^2+A_1x_1^2+A_2x_2^2 \tag{22}$$

with arbitrary A_1 and A_2.

(ii) Three-dimensional quartic anharmonic oscillator, $N=3$, $L=2$:

$$V\sim(x_1^2+x_2^2+x_3^2)^2+A_1x_1^2+A_2x_2^2+A_3x_3^2 \tag{23}$$

with arbitrary A_1, A_2 and A_3.

(iii) Two-dimensional sextic anharmonic oscillator, $N=2$, $L=3$:

$$V\sim(x_1^2+x_2^2)^3+(x_1^2+x_2^2)(A_1x_1^2+A_2x_2^2)+B_1x_1^2+B_2x_2^2 \tag{24}$$

with A_1, A_2, B_1 and B_2 such that

$$B_1-B_2=\tfrac{1}{4}(A_1^2-A_2^2). \tag{25}$$

(iv) Three-dimensional sextic anharmonic oscillator, $N=3$, $L=3$:

$$V\sim(x_1^2+x_2^2+x_3^2)^3+(x_1^2+x_2^2+x_3^2)(A_1x_1^2+A_2x_2^2+A_3x_3^2)+B_1x_1^2+B_2x_2^2+B_3x_3^2 \tag{26}$$

with A_1, A_2, A_3, B_1, B_2 and B_3 such that

$$B_i-B_k=\tfrac{1}{6}(A_i-A_k)[A_1+A_2+A_3+\tfrac{1}{2}(A_i-A_k)] \qquad i,k=1,2,3. \tag{27}$$

The more complex potentials in higher dimensions can also be obtained without difficulties. Note that in cases (i) and (ii) the separation of variables is permissible in coordinates λ for which $a_1-a_2=A_1-A_2$, while in cases (iii) and (iv) it is permissible in coordinates λ for which $a_i-a_k=\tfrac{1}{2}(A_i-A_k)$; $i,k=1,2,3$.

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