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Exact solution of the Schrödinger equation for a particle in a tetrahedral box

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Abstract. We obtain the exact solution of the Schrödinger equation for a particle confined to (i) an equilateral triangle, (ii) a tetrahedral box with corners $(-\pi/\sqrt{2}, -\pi/\sqrt{2}, -\pi/2)$, $(\pi/\sqrt{2}, -\pi/\sqrt{2}, \pi/2)$; $(-\pi/\sqrt{2}, \pi/\sqrt{2}, \pi/2)$ and $(\pi/\sqrt{2}, \pi/\sqrt{2}, -\pi/2)$. The energies are: for (i), $E_{nl} = (8\hbar^2\pi^2/9mL^2)(n^2 + l^2 - ln)$ where L is the side of the triangle and l, n are distinct non-zero integers and for (ii), $E_{lmn} = (\hbar^2/8m)\times[3(l^2+m^2+n^2) - 2lm - 2mn - 2nl]$ where l, m and n are distinct non-zero integers. The wavefunctions have been classified according to the irreducible representation of the corresponding symmetry groups.

1. Introduction

Exact solutions of the Schrödinger equation for a particle confined to certain regions of space (either two-dimensional or three-dimensional) have been found only for a few cases. We have found an amusing way to obtain the solution of the Schrödinger equation for: (i) a particle confined to an equilateral triangle in two dimensions; (ii) a particle confined in a tetrahedral box whose corners are $(-\pi/\sqrt{2}, -\pi/\sqrt{2}, -\pi/2)$, $(\pi/\sqrt{2}, -\pi/\sqrt{2}, \pi/2)$; $(-\pi/\sqrt{2}, \pi/\sqrt{2}, +\pi/2)$ and $(\pi/\sqrt{2}, \pi/\sqrt{2}, -\pi/2)$. Though (i) has been solved before using other methods, we believe that the results for the tetrahedral box are new. The solution to the problem is based on the Schrödinger equation of N hard cores confined to a length L in one dimension, the exact solution of which is known (Lieb and Mattis 1966). It is possible to transform the $N = 3$ and 4 cases of the hard-core problem into the problem of a single particle confined to a region in two and three dimensions respectively. It turns out that the region of confinement is an equilateral triangle for the two-dimensional case and a tetrahedron with corners specified as above for the case of three dimensions. To make the article self-contained, we reproduce the essential results of the N-hard-core problem in § 2. In § 3 we illustrate our method of transforming the equation of N hard cores to the Schrödinger equation of a single particle for the $N = 3$ case in detail. We then quote in § 4 the results for the $N = 4$ case. The wavefunctions have been classified according to the irreducible representations of the respective symmetry groups.

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2. Problem of N hard cores in one dimension

Consider N hard cores (molecules of vanishingly small length and mass m) whose coordinates x_i are confined to lie between 0 and L,

$$0 \leqslant x_i \leqslant L \qquad i = 1, 2, \ldots, n. \tag{2.1}$$

The cores are free to move in the allowed region and are to be treated as identical fermions. In particular, the wavefunction

$$\varphi(x_1 \ldots x_N) = 0 \tag{2.2}$$

whenever

$$x_i = x_j, \qquad i, j = 1, \ldots, N.$$

The Schrödinger equation

$$-\frac{\hbar^2}{2m} \sum_i \frac{\partial^2 \varphi}{\partial x_i^2} = E\varphi \tag{2.3}$$

with the above conditions (2.1) and (2.2), plus rigid boundary conditions has the following energy eigenvalues (Lieb and Mattis 1966):

$$En_1 \ldots n_N = (\hbar^2 \pi^2 / 2mL^2)(n_1^2 + n_2^2 + \ldots + n_N^2) \tag{2.4}$$

where n_i are distinct positive integers. The corresponding wavefunctions are the determinants

$$\underset{n_1 \ldots n_N}{\varphi(x_1 \ldots x_N)} = \begin{vmatrix} \sin k_1 x_1 & \sin k_1 x_2 & \ldots & \sin k_1 x_N \\ \vdots & & & \\ \sin k_N x_1 & \sin k_N x_2 & \ldots & \sin k_N x_N \end{vmatrix} \tag{2.5}$$

where $k_i = \pi n_i / L$.

We can state the same problem in terms of periodic boundary conditions, which is the form used in the present investigation. In this case the wavefunction obeys the boundary conditions (using coordinates θ_i in place of x_i):

$$\varphi(\theta_1, \ldots, \theta_j + 2\pi, \ldots, \theta_N) = \varphi(\theta_1, \ldots, \theta_j, \ldots, \theta_N) \qquad j = 1, \ldots, N \tag{2.6}$$

For these boundary conditions, the energy levels are

$$En_1 \ldots n_N = \frac{\hbar^2}{2m}(n_1^2 + n_2^2 + \ldots + n_N^2) \tag{2.7}$$

and the wavefunction is the determinant

$$\underset{n_1 \ldots n_N}{\varphi(\theta_1 \ldots \theta_N)} = \begin{vmatrix} \exp(in_1\theta_1) & \ldots & \exp(in_1\theta_N) \\ \exp(in_2\theta_1) & & \exp(in_2\theta_N) \\ \vdots & & \\ \exp(in_N\theta_1) & & \exp(in_N\theta_N) \end{vmatrix}. \tag{2.8}$$

3. Particle in an equilateral triangle

A useful transformation of the variables $\theta_1 \ldots \theta_N$ which allows us to separate the centre of mass of the whole system is

$$\begin{aligned} z_1 &= \theta_1 - \theta_2 \\ z_2 &= \tfrac{1}{2}(\theta_1 + \theta_2) - \theta_3 \\ &\vdots \\ z_i &= i^{-1}(\theta_1 + \ldots + \theta_i) - \theta_{i+1}, \qquad i \leqslant N-1 \\ &\vdots \\ z_N &= N^{-1}(\theta_1 + \ldots + \theta_N). \end{aligned} \tag{3.1}$$

The Schrödinger equation in terms of the new variables is

$$-\frac{\hbar^2}{2m}\left[2\frac{\partial^2}{\partial z_1^2} + \ldots + \frac{i+1}{i}\frac{\partial^2}{\partial z_i^2} + \ldots + \frac{N}{(N-1)}\frac{\partial^2}{\partial z_{N-1}^2} + \frac{1}{N}\frac{\partial^2}{\partial z_N^2}\right]\varphi = E\varphi. \tag{3.2}$$

For $N = 3$ these become

$$z_1 = \theta_1 - \theta_2 \qquad z_2 = \tfrac{1}{2}(\theta_1 + \theta_2) - \theta_3 \qquad z_3 = \tfrac{1}{3}(\theta_1 + \theta_2 + \theta_3) \tag{3.3}$$

and

$$-\frac{\hbar^2}{2m}\left[2\frac{\partial^2}{\partial z_1^2} + \frac{3}{2}\frac{\partial^2}{\partial z_2^2} + \frac{1}{3}\frac{\partial^2}{\partial z_3^2}\right]\varphi = E\varphi. \tag{3.4}$$

The z_3 coordinate describes motion associated with the centre of mass and the dependence of φ on it is separable. If we think of $(z_1/\sqrt{2})$ and $z_2\sqrt{2}/\sqrt{3}$ as the x and the y coordinates of a single particle, then we reproduce the Schrödinger equation for a single particle. However, the boundary conditions which were simple in terms of θ's have to be transformed in terms of new variables. Using

$$\begin{aligned} Y_1 &= z_1/\sqrt{2} = \tfrac{1}{2}(\theta_1 - \theta_2) \\ Y_2 &= z_2\sqrt{2}/\sqrt{3} = \sqrt{\tfrac{2}{3}}[\tfrac{1}{2}(\theta_1 + \theta_2) - \theta_3] \\ Y_3 &= \sqrt{3}z_3 = (\theta_1 + \theta_2 + \theta_3)/\sqrt{3}. \end{aligned} \tag{3.5}$$

We can find the restriction on the domain of the Y_1, Y_2 plane. To achieve this we invert equation (3.5) and get

$$\begin{aligned} \theta_1 &= Y_1/\sqrt{2} + Y_2/\sqrt{6} + Y_3/\sqrt{3} \\ \theta_2 &= -Y_1/\sqrt{2} + Y_2/\sqrt{6} + Y_3/\sqrt{3} \\ \theta_3 &= -2Y_2/\sqrt{6} + Y_3/\sqrt{3}. \end{aligned} \tag{3.6}$$

Without loss of generality, we can restrict the θ-space to the region $\theta_1 \geqslant \theta_2$, $\theta_2 \geqslant \theta_3$ and $\theta_3 + 2\pi \geqslant \theta_1$. In terms of the Y's these translate into the restrictions

$$Y_1 \geqslant 0, \qquad Y_1 \leqslant \sqrt{3}\,Y_2, \qquad Y_1/\sqrt{2} \leqslant 2\pi - Y_2\sqrt{\tfrac{3}{2}} \tag{3.7}$$

respectively. This corresponds to the particle being confined in an equilateral triangle with corners $(0, 0)$, $(\sqrt{2}\pi, \sqrt{\tfrac{2}{3}}\pi)$ and $(0, 2\sqrt{\tfrac{2}{3}}\pi)$. The wavefunction for the single particle can be obtained from equation (2.8) using the transformations (3.6).

$$\varphi(Y_1, Y_2, Y_3)_{n_1, n_2, n_3} = \begin{vmatrix} \exp\left[in_1\left(\frac{Y_1}{\sqrt{2}}+\frac{Y_2}{\sqrt{6}}+\frac{Y_3}{\sqrt{3}}\right)\right] & \exp\left[in_1\left(-\frac{Y_1}{\sqrt{2}}+\frac{Y_2}{\sqrt{6}}+\frac{Y_3}{\sqrt{3}}\right)\right] & \exp\left[+in_1\left(-\frac{2Y_2}{\sqrt{6}}+\frac{Y_3}{\sqrt{3}}\right)\right] \\ \exp\left[in_2\left(\frac{Y_1}{\sqrt{2}}+\frac{Y_2}{\sqrt{6}}+\frac{Y_3}{\sqrt{3}}\right)\right] & \exp\left[in_2\left(-\frac{Y_1}{\sqrt{2}}+\frac{Y_2}{\sqrt{6}}+\frac{Y_3}{\sqrt{3}}\right)\right] & \exp\left[in_2\left(-\frac{2Y_2}{\sqrt{6}}+\frac{Y_3}{\sqrt{3}}\right)\right] \\ \exp\left[in_3\left(\frac{Y_1}{\sqrt{2}}+\frac{Y_2}{\sqrt{6}}+\frac{Y_3}{\sqrt{3}}\right)\right] & \exp\left[in_3\left(-\frac{Y_1}{\sqrt{2}}+\frac{Y_2}{\sqrt{6}}+\frac{Y_3}{\sqrt{3}}\right)\right] & \exp\left[in_3\left(-\frac{2Y_2}{\sqrt{6}}+\frac{Y_3}{\sqrt{3}}\right)\right] \end{vmatrix}$$

$$= \exp[i(n_1+n_2+n_3)Y_3/\sqrt{3}]$$

$$\times \begin{vmatrix} 1 & 1 & 1 \\ \exp\left[i(n_2-n_1)\left(\frac{Y_1}{\sqrt{2}}+\frac{Y_2}{\sqrt{6}}\right)\right] & \exp\left[i(n_2-n_1)\left(-\frac{Y_1}{\sqrt{2}}+\frac{Y_2}{\sqrt{6}}\right)\right] & \exp\left[i(n_2-n_1)\left(-\frac{2Y_2}{\sqrt{6}}\right)\right] \\ \exp\left[i(n_3-n_1)\left(\frac{Y_1}{\sqrt{2}}+\frac{Y_2}{\sqrt{6}}\right)\right] & \exp\left[i(n_3-n_1)\left(-\frac{Y_1}{\sqrt{2}}+\frac{Y_2}{\sqrt{6}}\right)\right] & \exp\left[i(n_3-n_1)\left(-\frac{2Y_2}{\sqrt{6}}\right)\right] \end{vmatrix} \tag{3.8}$$

The factor $\exp[i(n_1+n_2+n_3)Y_3/\sqrt{3}]$ will be suppressed as it is separable and refers to the centre of mass motion of the three hard cores. We are interested only in the Y_1, Y_2 part. Writing

$$\phi_{l,m}(Y_1, Y_2) = \begin{vmatrix} 1 & 1 & 1 \\ \exp\left[il\left(\frac{Y_1}{\sqrt{2}}+\frac{Y_2}{\sqrt{6}}\right)\right] & \exp\left[il\left(-\frac{Y_1}{\sqrt{2}}+\frac{Y_2}{\sqrt{6}}\right)\right] & \exp\left[il\left(-\frac{2Y_2}{\sqrt{6}}\right)\right] \\ \exp\left[im\left(\frac{Y_1}{\sqrt{2}}+\frac{Y_2}{\sqrt{6}}\right)\right] & \exp\left[im\left(-\frac{Y_1}{\sqrt{2}}+\frac{Y_2}{\sqrt{6}}\right)\right] & \exp\left[im\left(-\frac{2Y_2}{\sqrt{6}}\right)\right] \end{vmatrix} \tag{3.9}$$

we immediately see that it satisfies the Schrödinger equation

$$-(\hbar^2/2m)[\partial^2/\partial Y_1^2+\partial^2/\partial Y_2^2]\phi_{l,m}(Y_1, Y_2) = E_{l,m}\phi_{l,m}(Y_1, Y_2) \tag{3.10}$$

with

$$E_{l,m} = (\hbar^2/3m)(l^2+m^2-lm). \tag{3.11}$$

This can either be obtained from

$$E_{n_1,n_2,n_3} = (\hbar^2/2m)(n_1^2+n_2^2+n_3^2) = (\hbar^2/2m)[\tfrac{1}{3}(n_1+n_2+n_3)^2+\tfrac{2}{3}(l^2+m^2-lm)]$$

and removing the centre of mass energy or by direct substitution of $\phi_{l,m}$ from equation (3.9) in equation (3.10).

For an equilateral triangle of side L, we will have the energy as

$$E_{l,m} = (8\hbar^2\pi^2/9mL^2)(l^2+m^2-lm) \tag{3.12}$$

and Y_i $(i=1,2)$ are to be interpreted as $(2\pi\sqrt{\tfrac{2}{3}}Y_i/L)$ in equation (3.9). This has been derived using other methods (Lame 1852, Mathews and Walker 1970).

We now discuss the symmetry of the solutions. It is clear that we have six symmetry operations under which the Schrödinger equation with the boundary conditions remains invariant, which form the group σ_{3v}.

We classify our solutions in terms of the irreducible representations A_1, A_2 and E of σ_{3v} (Landau and Lifshitz 1958). In order to do this it is more convenient to transform the Y_1, Y_2 coordinates so that the origin coincides with the centre of the triangle. We use

$$Y_1 = y_1 + \sqrt{2}\pi/3, \qquad Y_2 = y_2 + \sqrt{\tfrac{2}{3}}\pi \tag{3.13}$$

and write

$$\phi_{lm}(y_1, y_2) = \begin{vmatrix} 1 & 1 & 1 \\ \exp\left[\mathrm{i}l\left(\frac{y_1}{\sqrt{2}} + \frac{y_2}{\sqrt{6}} + \frac{2\pi}{3}\right)\right] & \exp\left[\mathrm{i}l\left(-\frac{y_1}{\sqrt{2}} + \frac{y_2}{\sqrt{6}}\right)\right] & \exp\left[-\mathrm{i}l\left(\frac{2y_2}{\sqrt{6}} + \frac{2\pi}{3}\right)\right] \\ \exp\left[\mathrm{i}m\left(\frac{y_1}{\sqrt{2}} + \frac{y_2}{\sqrt{6}} + \frac{2\pi}{3}\right)\right] & \exp\left[\mathrm{i}m\left(-\frac{y_1}{\sqrt{2}} + \frac{y_2}{\sqrt{6}}\right)\right] & \exp\left[-\mathrm{i}m\left(\frac{2y_2}{\sqrt{6}} + \frac{2\pi}{3}\right)\right] \end{vmatrix} \tag{3.14}$$

The operation of C_3 and σ_v in terms of y_1 and y_2 are

$$C_3: \qquad y_1 \to -\tfrac{1}{2}(y_1 - \sqrt{3}y_2) \qquad y_2 \to -\tfrac{1}{2}(\sqrt{3}y_1 + y_2) \tag{3.15}$$

and

$$\sigma_v: \qquad y_1 \to y_1 \qquad y_2 \to -y_2.$$

It is easy to verify that

$$C_3\phi_{lm} = \exp[\mathrm{i}\tfrac{2}{3}\pi(l+m)]\phi_{lm}$$

and

$$\sigma_v\phi_{lm} = -\exp[\mathrm{i}\tfrac{2}{3}\pi(l+m)]\phi^*_{lm}. \tag{3.16}$$

It immediately follows that, if $l+m = 3p$ where p is an integer

$\frac{1}{2}(\phi_{lm} - \phi^*_{lm})$ transforms as A_1 and

$\frac{1}{2}(\phi_{lm} + \phi^*_{lm})$ transforms as A_2.

On the other hand, if $l+m = 3p+1$ or $3p+2$, ϕ_{lm} and $\phi^*_{l,m}$ form a basis for the irreducible representation E.

4. Particle in a tetrahedron

The procedure which leads to the solution of a particle in a tetrahedron with corners A $(-\pi/\sqrt{2}, -\pi/\sqrt{2}, -\pi/2)$; B $(\pi/\sqrt{2}, -\pi/\sqrt{2}, \pi/2)$; C $(-\pi/\sqrt{2}, \pi/\sqrt{2}, \pi/2)$ and D $(\pi/\sqrt{2}, \pi/\sqrt{2}, -\pi/2)$ is similar to the one described in the previous section. Here we work with the $N=4$ solution of equation (2.8). We will not repeat all the details, but only write down some of the relevant steps and the final results. The transformations are

$$\begin{aligned} \theta_1 &= \tfrac{1}{2}y_4 + \tfrac{1}{2}y_3 + \tfrac{1}{2}y_1\sqrt{2} + \tfrac{3}{4}\pi & \theta_2 &= \tfrac{1}{2}y_4 - \tfrac{1}{2}y_3 + \tfrac{1}{2}y_2\sqrt{2} + \tfrac{1}{4}\pi \\ \theta_3 &= \tfrac{1}{2}y_4 + \tfrac{1}{2}y_3 - \tfrac{1}{2}y_1\sqrt{2} - \tfrac{1}{4}\pi & \theta_4 &= \tfrac{1}{2}y_4 - \tfrac{1}{2}y_3 - \tfrac{1}{2}y_2\sqrt{2} - \tfrac{3}{4}\pi. \end{aligned} \tag{4.1}$$

The conditions $\theta_1 \geqslant \theta_2$, $\theta_2 \geqslant \theta_3$, $\theta_3 \geqslant \theta_4$ and $\theta_4 + 2\pi \geqslant \theta_1$ lead to the particle being confined in the tetrahedron ABCD in the y_1, y_2, y_3 space. The wavefunction after removing the centre of mass coordinate is the 4×4 determinant

$$\phi_{lmn}(y_1, y_2, y_3) = \begin{vmatrix} 1 & 1 & 1 & 1 \\ \exp\left[il\left(\frac{y_1}{\sqrt{2}}+\frac{y_3}{2}+\frac{3\pi}{4}\right)\right] & \exp\left[il\left(\frac{y_2}{\sqrt{2}}-\frac{y_3}{2}+\frac{\pi}{4}\right)\right] & \exp\left[il\left(-\frac{y_1}{\sqrt{2}}+\frac{y_3}{2}-\frac{\pi}{4}\right)\right] & \exp\left[il\left(-\frac{y_2}{\sqrt{2}}-\frac{y_3}{2}-\frac{3\pi}{4}\right)\right] \\ \exp\left[im\left(\frac{y_1}{\sqrt{2}}+\frac{y_3}{2}+\frac{3\pi}{4}\right)\right] & \exp\left[im\left(\frac{y_2}{\sqrt{2}}-\frac{y_3}{2}+\frac{\pi}{4}\right)\right] & \exp\left[im\left(-\frac{y_1}{\sqrt{2}}+\frac{y_3}{2}-\frac{\pi}{4}\right)\right] & \exp\left[im\left(-\frac{y_2}{\sqrt{2}}-\frac{y_3}{2}-\frac{3\pi}{4}\right)\right] \\ \exp\left[in\left(\frac{y_1}{\sqrt{2}}+\frac{y_3}{2}+\frac{3\pi}{4}\right)\right] & \exp\left[in\left(\frac{y_2}{\sqrt{2}}-\frac{y_3}{2}+\frac{\pi}{4}\right)\right] & \exp\left[in\left(-\frac{y_1}{\sqrt{2}}+\frac{y_3}{2}-\frac{\pi}{4}\right)\right] & \exp\left[in\left(-\frac{y_2}{\sqrt{2}}-\frac{y_3}{2}-\frac{3\pi}{4}\right)\right] \end{vmatrix} \tag{4.2}$$

the energy is

$$E_{lmn} = (\hbar^2/8m)[3(l^2+m^2+n^2) - 2lm - 2ln - 2mn)]. \tag{4.3}$$

The corners of the tetrahedron have been chosen so that the line joining the mid points of AC and BD is the y_1 axis, that joining the mid points of AB and CD is the y_2 axis, and that joining the mid points of AD and BC is the y_3 axis. The tetrahedron goes into itself (see figure 1) under:

(i) Identity (O_1),
(ii) rotation of π about y_1 axis (O_2),
(iii) rotation of π about y_2 axis (O_3),
(iv) rotation of π about y_3 axis (O_4),
(v) reflection in the plane $y_1 = y_2$ (O_5),
(vi) reflection in the plane $y_1 + y_2 = 0$ (O_6),
(vii) rotation of $\frac{1}{2}\pi$ about the y_3 axis followed by reflection in the plane $y_3 = 0$ (O_7),
(viii) rotation of $-\frac{1}{2}\pi$ about the y_3 axis followed by reflection in the plane $y_3 = 0$ (O_8).

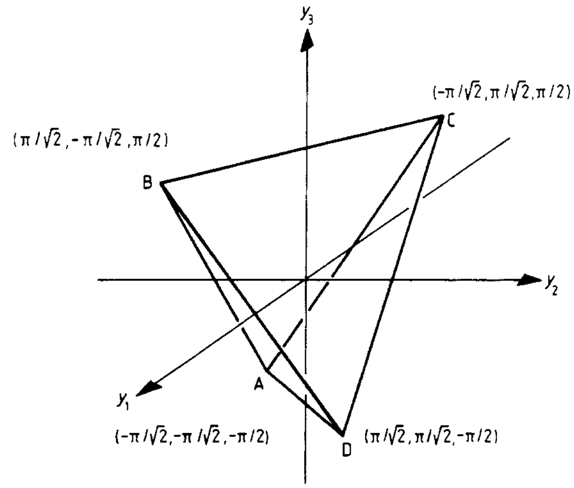

Figure 1. Geometry of the tetrahedral box for which (4.2) gives the eigenfunctions of the Schrödinger equation.

The operations form an eight-element group D_{2d}. The irreducible representations are classified as A_1, A_2, B_1, B_2 and E (Landau and Lifshitz 1958). One also has

$$O_2\phi_{lmn} = -\exp[i(l+m+n)\tfrac{1}{2}\pi]\phi^*_{lmn}$$

$$O_3\phi_{lmn} = -\exp[-i(l+m+n)\tfrac{1}{2}\pi]\phi^*_{lmn}$$

$$O_4\phi_{lmn} = \exp[i(l+m+n)\pi]\phi_{lmn}$$

$$O_5\phi_{lmn} = \phi^*_{lmn}$$

$$O_6\phi_{lmn} = \exp[i(l+m+n)\pi]\phi^*_{lmn}$$

$$O_7\phi_{lmn} = -\exp[i(l+m+n)\tfrac{1}{2}\pi]\phi_{lmn}$$

$$O_8\phi_{lmn} = -\exp[-i(l+m+n)\tfrac{1}{2}\pi]\phi_{lmn}.$$

These can be used to determine the symmetry properties of the wavefunctions. In particular,

(i) for $l+m+n=4p$, where p is an integer, the wavefunction $(\phi_{l,m,n}-\phi^*_{l,m,n})$ belongs to the representation B_1 and $(\phi_{l,m,n}+\phi^*_{l,m,n})$ belongs to B_2;

(ii) for $l+m+n=4p+1$, $4p+3$; $\phi_{l,m,n}$ and $\phi^*_{l,m,n}$ form the basis for the two-dimensional representation E; and finally

(iii) for $l+m+n=4p+2$; $(\phi_{lmn}+\phi^*_{lmn})$ belongs to A_1 and $(\phi_{l,m,n}-\phi^*_{l,m,n})$ belongs to the representation A_2.

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