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On the quantum particle in a polyhedral box

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Abstract. The recently obtained solution of the Schrödinger equation for a particle confined to a particular (non-regular) tetrahedral box is rederived directly rather than through a transformation of a four-body one-dimensional problem. Its simple form is shown to be related to a space-filling property of this particular tetrahedron. The class of all such polyhedra is determined.

1. Introduction

Among all orthogonal coordinate systems, it is only in the case of confocal surfaces of the second degree that the method of separation of variables can be applied to solving the eigenvalue problem

$$\Delta u + k^2 u = 0, \tag{1.1}$$

Δ being the n-dimensional Laplacian (Weber 1869).

Only two cases not involving such a separation of variables have apparently been solved, namely when the boundary is an equilateral triangle (Lamé 1852) and quite recently, when it is a particular tetrahedron (with Dirichlet boundary conditions) (Krishnamurthy *et al* 1982).

In the latter case, the authors recovered Lamé's result through an ingenious mapping of a one-dimensional three-body problem (hard core fermions on a segment) into a one-body problem within a two-dimensional region which turned out to be an equilateral triangle. The spectrum was shown to be proportional to the quadratic form $l^2 - lm + m^2$, where l, m are integers subject to three conditions ($l \neq 0$, $m \neq 0$ and $l \neq m$) which guarantee that the wavefunction, written as a 3×3 Slater determinant does not vanish identically.

When applied to a similar four-body problem, the mapping leads to a one-body problem within a tetrahedron (referred to hereafter as the K tetrahedron) having two opposite edges equal to 1 and the remaining four equal to $3^{1/2}/2$. The spectrum in this case is proportional to the quadratic form $3l^2+3m^2+3n^2-2lm-2mn-2nl$, where the three integers l, m and n are subject to six conditions: l, m and n all $\neq 0$ and distinct. There are six conditions because the wavefunction is now a 4×4 Slater determinant which vanishes if any pair of rows, of which there are $C_4^2 = 6$, is identical. Thus in both cases where no separation of variables is involved, the solution of (1.1) is expressible as a *finite* sum of the form

$$\sum_j c_j \exp(\mathrm{i}\bar{k}_j \cdot \bar{r}) \tag{1.2}$$

Furthermore, whereas the three-body problem leads to the solution of the equilateral (i.e. the most symmetrical) triangle case, the four-body problem leads to the solution of a non-regular tetrahedral problem. What geometrical properties of the equilateral triangle and of the K tetrahedron (not apparently shared by the regular tetrahedron) make it possible to solve (1.1) in the form of a finite sum (1.2), and can these results be obtained directly rather than through a transformation of a seemingly unrelated problem? Do other polygons and polyhedra share this property?

2. Riemann–Schwarz reflexion principle

The solution of $\Delta u + k^2 u = 0$, $u \in D$ (a bounded region) and $u|_{\delta D} = 0$, can be continued beyond D, when its boundary δD contains a line segment, by reflection: let P' be the mirror image with respect to this segment of a point $P \in D$, and let $u(P') = -u(P)$. In this way the solution of equation (1.1) inside D is extended into the mirror image D' of D, and a solution $\varepsilon\ C_2$ in the combined domain $D + D'$ is thus obtained (Courant 1918, Courant and Hilbert 1953).

If D is a polygon, the solution inside D can be extended around any vertex by repeated reflections; but if this solution is expressible inside D as a finite sum (1.2), then clearly this sum also represents the solution in the whole plane. Therefore an even number of reflections around any given vertex of the polygon must bring it back into coincidence with itself. Each angle of the polygon must equal $2\pi/2p$, p an integer $\geqslant 2$.

This necessary condition alone reduces the number of possible cases to four. Firstly let D be a triangle and $\alpha_i = 2\pi/2p_i$ ($p_i \geqslant 2$, $i = 1, 2, 3$) its angles. As $\Sigma\ 1/p_i = 1$, the only possible values for (p_1, p_2, p_3), to within permutations, are $(3, 3, 3)$, $(2, 3, 6)$ and $(2, 4, 4)$, i.e. respectively the equilateral triangle, a harmonic of the equilateral triangle, and a harmonic of the square. Secondly let D be a quadrilateral; the only solution of $\Sigma\ 1/p_i = 2$ is $p_1 = p_2 = p_3 = p_4 = 2$, i.e. D is a rectangle. Polygons with a number of sides greater than four are excluded.

It will be shown in the next paragraph that in these cases the solution to equation (1.1) with Dirichlet boundary conditions is indeed expressible in the finite form (1.2).

The same argument can be applied to the three-dimensional case. There must be an even number of reflections of the polyhedron, with respect to a face, around any edge which brings it into coincidence with itself, and so each dihedral angle δ_i must equal $2\pi/2p_i$, p_i an integer $\geqslant 2$.

Now the dihedral angles of a trihedral angle are subject to strict inequalities: $3\pi > \delta_1 + \delta_2 + \delta_3 > \pi$, thus $\Sigma\ 1/p_i > 1$, and therefore for the n dihedral angles of an n-hedral angle, $\Sigma\ 1/p_i > n - 2$. This immediately implies that at each vertex exactly three edges meet, for should there be more, say n, then the inequality $\Sigma\ 1/p_i > n - 2$, $p_i \geqslant 2$, $n > 3$ cannot be satisfied.

Consequently all faces of the polyhedron are necessarily triangles or rectangles: indeed let δ_i be the dihedral angles and α_i the opposite face angles at some vertex, and recall that $\cos \delta_i = (\cos \alpha_i - \cos \alpha_j \cos \alpha_k)/\sin \alpha_j \sin \alpha_k$, ($i, j, k$ a permutation of 1, 2, 3). Now $0 < \delta_i \leqslant \pi/2$ and $0 < \alpha_i < \pi$ ($i = 1, 2, 3$) imply $\cos \delta_i \geqslant 0$ and $\sin \alpha_i > 0$. Therefore $\cos \alpha_i \geqslant \cos \alpha_j \cos \alpha_k$, and this in turn implies $0 < \alpha_i \leqslant \pi/2$. If D has a face with n sides, the sum of its face angles will be $\leqslant n\pi/2$. On the other hand this must be $(n-2)\pi$, therefore $n = 3$ or 4 (and in the latter case each face angle is necessarily $\pi/2$.)

Let E, V and F be respectively the number of edges, vertices and faces of the polyhedron D. As $2E = 3V$, V is necessarily even; it cannot be greater than 8, for assume $V \doteq 2v > 8$, then $E = 3v > 12$, and $F = E - V + 2 = v + 2 > 6$. If there are F_3 and F_4 triangular and rectangular faces, then $F_3 + F_4 = F = v + 2$, and $3F_3 + 4F_4 = 2E = 6v$, whence $F_3 = 8 - 2v < 0$.

If $V = 8$, $E = 12$, $F = 6$ and $F_3 = 0$, $F_4 = 6$: D is a rectangular parallelepiped, a case completely soluble by separation of variables.

If $V = 6$, $E = 9$, $F = 5$ and $F_3 = 2$, $F_4 = 3$; it is easy to see that the two triangular faces cannot be contiguous, so that D is a rectangular prism with triangular base, and by separation of variables it follows that this triangle must be one of the three considered in the two-dimensional case.

If $V = 4$, $E = 6$, $F = 4$ and $F_3 = 4$; D is a tetrahedron and this case requires detailed analysis: the six dihedral angles are subject to four inequalities of the form $\Sigma\, \delta_i > \pi$. They imply that at *least* two of these angles must be right angles. If there are exactly two, they belong to opposite edges. The various inequalities reduce the number of possible values for the remaining four dihedrals to a sufficiently small number (eleven) for a systematic search to be envisaged: it is found that the only compatible case is when the remaining dihedrals are all equal to $\pi/3$, which is precisely the case of the K tetrahedron.

If there are three right angle dihedrals, either (i) they belong to concurrent edges in which case it turns out that the remaining angles are $\pi/3$, $\pi/3$ and $\pi/4$, or (ii) if not the remaining angles are $\pi/3$, $\pi/4$ and $\pi/4$. Both of these tetrahedra are harmonics of the K tetrahedron, which has two symmetry planes, one through each long edge and the mid-point of the opposite long edge. Each plane splits the K tetrahedron into two tetrahedra of type (i). The two together split it into four tetrahedra of type (ii).

These tetrahedra (i) and (ii) lead to tessellations not only of the K tetrahedron but also of the cube, which requires twelve of type (i) and twenty four of type (ii); this implies that the K tetrahedron and the cube share a common subset of their spectrum. Indeed the former with sides $\{1^2, (\frac{1}{2}\surd 3)^4\}$ has as spectrum

$$\begin{aligned} \lambda^K_{lmn} &= \pi^2(3l^2 + 3m^2 + 3n^2 - 2lm - 2mn - 2nl) \\ &= \pi^2\{(-l + m + n)^2 + (l - m + n)^2 + (l + m - n)^2\} \end{aligned}$$

and the latter (edges equal to 1)

$$\lambda^C_{pqr} = \pi^2(p^2 + q^2 + r^2),$$

where l, m and n are distinct non-zero integers, and p, q and r are non-zero integers. As $(-l + m + n)$ for example can equal zero,

$$\{\lambda^K_{lmn}\} \not\subset \{\lambda^C_{pqr}\}.$$

Conversely not every choice of p, q and r leads to acceptable values for l, m and n:

$$\{\lambda^K_{lmn}\} \not\supset \{\lambda^C_{pqr}\}.$$

However, values of p, q and r that do lead to acceptable values for l, m and n have necessarily same parity. If all odd, then for the cube the wavefunction

$$(\tfrac{1}{6})^{\frac{1}{2}} \sum \varepsilon_{ijk} u_i(x) u_j(y) u_k(z)$$

where ε_{ijk} is the completely antisymmetric tensor, the sum carries over all permutations of (p, q, r) and the functions u are solutions of equation (1.1) in one dimension, has nodal planes through the six pairs of opposite edges of the cube and splits into twelve tetrahedra of type (i). If p, q and r are all even, then there are three additional nodal planes through the mid-points of parallel edges, and these planes together with the six previous ones split the cube into twenty four tetrahedra of type (ii).

3. Explicit solution for the equilateral triangle and K tetrahedron

Let two lines $kx+ly+m=0$ and $k'x+l'y+m'=0$ be mirror images with respect to a third line $ax+by+c=0$, then

$$\begin{pmatrix} k' \\ l' \end{pmatrix} = \frac{1}{a^2+b^2}\begin{pmatrix} a^2-b^2 & 2ab \\ 2ab & -a^2+b^2 \end{pmatrix}\begin{pmatrix} k \\ l \end{pmatrix} \doteq R_{ab}\begin{pmatrix} k \\ l \end{pmatrix}. \tag{3.1}$$

For an equilateral triangle ABC, with vertices at $A(0,0)$, $B(1,0)$ and $C(\frac{1}{2},\frac{1}{2}\sqrt{3})$, let

$$R_1 \doteq R_{BC} = \begin{pmatrix} \frac{1}{2} & \frac{1}{2}\sqrt{3} \\ \frac{1}{2}\sqrt{3} & -1 \end{pmatrix}, \qquad R_2 \doteq R_{AB} = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix},$$

$$R_3 \doteq R_{AC} = \begin{pmatrix} \frac{1}{2} & -\frac{1}{2}\sqrt{3} \\ -\frac{1}{2}\sqrt{3} & -\frac{1}{2} \end{pmatrix}.$$

If the solution of equation (1.1) can be expressed in the form (1.2) and if $\binom{p}{q}$ is a direction appearing in the sum, then all directions obtained by multiple reflections must also appear. In the case of the equilateral triangle, these reflections generate a group of order six: $\{E \doteq R_0, R_1, R_2, R_3, R_1R_2, R_2R_1\}$. It is simply the symmetry group of the equilateral triangle and is isomorphic to the symmetric group of degree three.

Thus $u(x,y)$, if it can be expressed in the form (1.2), must be of the form

$$u(x,y) = \sum_0^5 a_j \exp\left[\mathrm{i}\,(p\;q)\,R_j^T\begin{pmatrix} x \\ y \end{pmatrix}\right] + \mathrm{cc}. \tag{3.2}$$

Imposing the boundary condition $u=0$ on sides AB and AC shows that

$$a_0 = -a_1^* = -a_2^* = -a_3^* = a_4 = a_5,$$

and $u=0$ on side BC leads to three conditions

$$\exp(\mathrm{i}q\sqrt{3}) - \exp[-\mathrm{i}(3p-q\sqrt{3})/2] = 0$$

$$\exp(\mathrm{i}q\sqrt{3}) - \exp[\mathrm{i}(3p+q\sqrt{3})/2] = 0$$

$$\exp[-\mathrm{i}(3p+q\sqrt{3})/2] - \exp[-\mathrm{i}(3p-q\sqrt{3})/2 = 0.$$

These three conditions on p and q turn out to be compatible and are satisfied if

$$p = (2\pi/3)(2r+s), \qquad q = (2\pi/\sqrt{3})s$$

with r and s integers. In this case therefore the solution can indeed be expressed in the form (1.2) and the spectrum is given by

$$\lambda_{rs} = p^2(r,s) + q^2(r,s) = \tfrac{16}{9}\pi^2(r^2+rs+s^2),$$

which is Lamé's expression.

To recover the quadratic form as given by Krishnamurthy *et al* (1982) we simply write

$$r^2+rs+s^2 = (r+s)^2 - (r+s)s + s^2 \equiv l^2 - lm + m^2.$$

Now the values of r and s are subject to the following conditions: should the direction $\binom{p}{q}$ be perpendicular to any of the three sides of the triangle, then the line will be reflected back upon itself, cancel out and lead to a vanishing wavefunction. Thus each scalar product of $\binom{p}{q}$ with $\binom{0}{1}$, $\binom{\pm\sqrt{3}}{1}$ must be different from zero.

Therefore $q \neq 0$ and $\pm\sqrt{3}\, p + q \neq 0$, and in terms of r and s

$$r \neq 0, \qquad s \neq 0, \qquad r + s \neq 0,$$

so finally l and m must be non-zero distinct integers, which are exactly the restrictions found by Krishnamurthy *et al.*

The above construction is readily extended to the K tetrahedron. Let two planes $kx + ly + mz + n = 0$ and $k'x + l'y + m'z + n' = 0$ be mirror images with respect to a third plane $ax + by + cz + d = 0$. Then

$$\begin{pmatrix} k' \\ l' \\ m' \end{pmatrix} = \frac{1}{a^2+b^2+c^2} \begin{pmatrix} a^2-b^2-c^2 & 2ab & 2ac \\ 2ab & -a^2+b^2-c^2 & 2bc \\ 2ac & 2bc & -a^2-b^2+c^2 \end{pmatrix} \begin{pmatrix} k \\ l \\ m \end{pmatrix}.$$

For convenience we place the vertices of the tetrahedron at $A(1, 0, -\sqrt{2})$, $B(2, 0, 0)$, $C(0, 0, 0)$ and $D(1, -\sqrt{2}, 0)$. The reflection matrices for the four faces are

$$R_1 \doteq R_{ABD} = \begin{pmatrix} 0 & -\alpha & -\alpha \\ -\alpha & -\alpha^2 & \alpha^2 \\ -\alpha & \alpha^2 & -\alpha^2 \end{pmatrix}, \qquad R_2 \doteq R_{ABC} = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

$$R_3 \doteq R_{BCD} = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \qquad R_4 \doteq R_{ACD} = \begin{pmatrix} 0 & \alpha & \alpha \\ \alpha & -\alpha^2 & \alpha^2 \\ \alpha & \alpha^2 & -\alpha^2 \end{pmatrix}$$

where $\alpha = \frac{1}{2}\sqrt{2}$.

Multiple reflections in this case lead to a group of order twenty four which is isomorphic to the full symmetry group T_d of the regular tetrahedron, and is generated by

$R_0 = E$	$R_6 = 341$	$R_{12} = 12$	$R_{18} = 343$
R_1	$R_7 = 13$	$R_{13} = 24$	$R_{19} = 321$
R_2	$R_8 = 31$	$R_{14} = 42$	$R_{20} = 324$
R_3	$R_9 = 43$	$R_{15} = 213$	$R_{21} = 32$
R_4	$R_{10} = 34$	$R_{16} = 243$	$R_{22} = 41$
$R_5 = 241$	$R_{11} = 21$	$R_{17} = 313$	$R_{23} = 3241$

where e.g. xyz stands for $R_x R_y R_z$.

With this labelling, the isomorphism with T_d is given explicitly as follows (Landau and Lifshitz 1958)

$R_0 = E$		
R_1 *to* R_6	σ_d	(six reflections)
R_7 to R_{14}	C_3, C_3^2	(eight rotations)

R_{15} to R_{20} $\quad S_4, S_4^3 \quad$ (six reflection–rotations)

R_{21} to R_{23} $\quad C_2(=S_4^2) \quad$ (three rotations).

We write

$$u(x, y, z) = \sum_0^{23} a_j \exp\left\{ \mathrm{i}\, \underbrace{p\, q\, r}\, R_j^T \begin{pmatrix} x \\ y \\ z \end{pmatrix} \right\} + \mathrm{cc}$$

and impose Dirichlet boundary conditions on the three faces passing through $C(0, 0, 0)$: it turns out that if R_i is a rotation, then $a_i = \alpha$, and if R_i is a reflection or a reflection–rotation, then $a_i = \beta$ with $\alpha = -\beta^*$. The remaining boundary condition on the fourth face (ABD) leads to the twelve congruences

$$\underbrace{p\, q\, r}\, (R_k^T + R_{k'}^T) \begin{pmatrix} 0 \\ 0 \\ \sqrt{2} \end{pmatrix} \equiv 0 \qquad (2\pi)$$

where R_k is any one of the twelve rotations and $R_k{}' = R_1 R_k$.

All these congruences are satisfied if

$$p = \frac{2\rho\pi}{4}, \qquad q = \frac{2\sigma\pi}{2\sqrt{2}}, \qquad r = \frac{2\tau\pi}{2\sqrt{2}},$$

where ρ, σ and τ are integers and $\rho + \sigma - \tau$ must be even. Consequently the spectrum is given by

$$\lambda_{\rho\sigma\tau} = p^2 + q^2 + r^2 = \tfrac{1}{4}\pi^2(\rho^2 + 2\sigma^2 + 2\tau^2).$$

As in the triangular case, these integers ρ, σ and τ are subject to the condition that the direction $\begin{bmatrix} p \\ q \\ r \end{bmatrix}$ not be perpendicular to any of the planes of the faces of the tetrahedron or any of the reflected planes. As filling space through repeated reflections of this tetrahedron is equivalent to slicing space with six infinite sets of planes parallel respectively to

$$\begin{array}{ll} & \sqrt{2}x - y + z = 0 \\ y = 0 & \sqrt{2}x + y - z = 0 \\ z = 0 & -\sqrt{2}x + y + z = 0 \\ & \sqrt{2}x + y + z = 0 \end{array}$$

the scalar product of $\begin{bmatrix} \rho \\ q \\ r \end{bmatrix}$ with any of the following:

$$\begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix}, \quad \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}, \quad \begin{bmatrix} \sqrt{2} \\ -1 \\ 1 \end{bmatrix}, \quad \begin{bmatrix} \sqrt{2} \\ 1 \\ -1 \end{bmatrix}, \quad \begin{bmatrix} -\sqrt{2} \\ 1 \\ 1 \end{bmatrix}, \quad \begin{bmatrix} \sqrt{2} \\ 1 \\ 1 \end{bmatrix}$$

must not vanish.

In terms of ρ, σ and τ this implies

$$\sigma \neq 0, \qquad \tau \neq 0, \qquad \rho - \sigma + \tau \neq 0, \qquad \rho + \sigma - \tau \neq 0,$$

$$-\rho + \sigma + \tau \neq 0, \qquad \rho + \sigma + \tau \neq 0.$$

To recover the Krishnamurthy form for the spectrum, put

$$\rho = -l + m + n, \qquad \sigma = l, \qquad \tau = -m + n.$$

Then

$$p^2 + 2\sigma^2 + 2\tau^2 = 3l^2 + 3m^2 + 3n^2 - 2lm - 2mn - 2nl,$$

and the six conditions on p, σ and τ yield respectively

$$l \neq 0, \qquad m \neq n, \qquad l \neq n, \qquad m \neq 0, \qquad l \neq m, \qquad n \neq 0.$$

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