Geometrical description of the convex sets of states for systems with spin-1/2 and spin-1

1976 J. Phys. A: Math. Gen. 9 2059

(http://iopscience.iop.org/0305-4470/9/12/011)

J. Phys. A: Math. Gen., Vol. 9, No. 12, 1976. Printed in Great Britain. © 1976

Geometrical description of the convex sets of states for systems with spin-$\frac{1}{2}$ and spin-1

F J Bloore†

Department of Physics, Dalhousie University, Halifax, Nova Scotia, Canada, B3H 3J5

Received 7 April 1976

Abstract. The states of a quantum mechanical system form a convex set with the pure states as extremals. For a system of spin-$\frac{1}{2}$, the set is a 3-dimensional ball. For spin j, the convex set is stratified by rank r, $1 \leq r \leq 2j+1$. The dimension of the stratum of rank r is $r[2(2j+1)-r]-1$. We describe geometrically, for $j=1$, how the strata with $r=1, 2, 3$ fit together in the 8-dimensional convex set. As a simpler example, we give the real section of this set, i.e., we describe the states of the real 3×3 matrix algebra.

1. Introduction

This paper offers a geometrical description of the convex set of states for a spin-$\frac{1}{2}$ and for a spin-1 quantum system. The purpose is pedagogical; the descriptions probably have no direct usefulness, but they illustrate aspects of the convexity property of states which is now an important concept in statistical mechanics. It is hoped that this account will be a helpful complement to the algebraic specification of spin states given by Park and Band (1971). The convexity of the set of states of a general quantum system was first discussed by Segal (1947). We shall discuss only the states of a system having a finite-dimensional Hilbert space. Such states are elements of a closed bounded convex subset of a finite-dimensional real vector space. Henceforth we restrict our discussion to this sort of convex set.

In § 2 we show that such convex sets are stratified by rank. A point of a convex set is *extremal* if it is not a convex combination of two other points. The *rank* of a point of a convex set is the minimal number of extremal points of which it is a convex combination and is well defined in the sets as restricted above. States of a quantum mechanical system are specified by density operators. In § 3 we show that these form a convex set and that the rank of a density operator is its rank in vector space terminology, namely the dimension of its range. The pure states have rank one and are the extremal points of the set.

In a convex set, the set of points of maximal rank has maximal dimension and forms the interior of the set. The interior is surrounded by a hierarchy of hyperfaces of all lower ranks down to one. In the simplest convex sets, the dimension of a stratum of a given rank drops by one as the rank drops by one. For example, the three-dimensional tetrahedron has an interior of rank 4, faces of rank 3, edges of rank 2, and vertices of

†Senior Killam Fellow, 1975–76. Permanent address: DAMTP, The University, Liverpool L69 3BX, UK

rank 1. The three-dimensional ball has an interior of rank 2 and a surface of rank 1. However, as we show in § 4, the dimension of the set of states of rank $r \leqslant 2j+1$ of a spin-j system is $r[2(2j+1)-r]-1$, which is a nonlinear function of rank. This is the motivation to see geometrically precisely how the pure states and the mixed states of different ranks are positioned relative to each other in the convex set of states. We exhibit these sets for a spin-$\frac{1}{2}$ system and a spin-1 system in §§ 5 and 6. The spin-$\frac{1}{2}$ set is too simple to show the general features and the spin-1 set has too many dimensions to be satisfactorily imaginable, so in § 7 we describe the 'real slice' of the spin-1 set; this has fewer dimensions and is more accessible to the imagination.

2. Convex sets

We begin by stating some standard results (Eggleston 1969). Let S be a closed bounded subset of a finite-dimensional real vector space. We say S is *convex* if given any two points x, y of S, the points

$$\lambda x+(1-\lambda)y, \qquad 0\leqslant\lambda\leqslant 1$$

of the line between them all lie in S. A point $z\in S$ is called *extremal* if it has no such decomposition into other points x, y of S. Extremal points of S exist. Any point x of S may be expressed as a *convex combination* of extremal points, i.e.,

$$x=\sum_{i=1}^{r}\lambda_i z_i, \qquad \lambda_i\geqslant 0, \qquad \sum_i \lambda_i=1,$$

where the z_i are extremal. This expression is not usually unique. The *rank* of x is the smallest number r of the z_i needed. Thus the extremal points have rank one, and the rank function divides the set into strata which are connected subsets of points of equal rank.

3. Density operators

We consider a quantum mechanical system whose observables are the Hermitian elements $A=A^*$ of the set $L(\mathscr{H})$ of linear operators on a complex Hilbert space $\mathscr{H}$ of finite dimension n. A *state* ω of the system is a normalized positive linear functional on $L(\mathscr{H})$, i.e.,

$$\omega: L(\mathscr{H})\rightarrow\mathbb{C},$$

$$\text{(i)} \quad \omega(1)=1, \quad \text{(normalization)}$$

$$\text{(ii)} \quad \omega(A^*A)>0 \quad \text{if } A\neq 0, \quad \text{(positivity)}$$

$$\text{(iii)} \quad \omega(c_1A_1+c_2A_2)=c_1\omega(A_1)+c_2\omega(A_2), \quad \text{(linearity)}.$$

It follows that if $A=A^*$ then $\omega(A)$ is real. We may write $L(\mathscr{H})=\mathscr{H}\otimes\mathscr{H}'$, where $\mathscr{H}'$ is the dual vector space of $\mathscr{H}$; the set of states is the positive subset of the dual of this set (which is actually self-dual). Thus states are also elements of $L(\mathscr{H})$, and the action is $\omega(A)=\mathrm{Tr}(\omega\,.\,A)$. The conditions (i) and (ii) require the states to be positive Hermitian elements of $L(\mathscr{H})$ with unit trace. So regarded, the states are usually called *density operators*. Evidently any convex sum of density operators is another density operator, so the states form a convex set. Since any density operator ω is Hermitian it may be diagonalized into a sum of projections $|\lambda_i\rangle\langle\lambda_i|$ onto its (orthogonal) eigenspaces, where the coefficients are the eigenvalues λ_i,

$$\omega=\sum_{i=1}^{n}\lambda_i|\lambda_i\rangle\langle\lambda_i|. \tag{1}$$

Since ω is positive and of unit trace, this is a convex decomposition. No projection operator $|\lambda_i\rangle\langle\lambda_i|$ can be further decomposed, and so these form the extremal points of the convex set. To each element $|\psi\rangle\in\mathscr{H}$ there corresponds the density operator $|\psi\rangle\langle\psi|$; this is usually called a pure state. We see that the 'vector space' rank of ω equals the 'convex set' rank of ω, since both are equal to the number of terms on the right-hand side of equation (1).

4. Dimension of space of $n\times n$ Hermitian operators of rank r

We first compute the number of degrees of freedom in an $n\times n$ Hermitian matrix whose first r columns are linearly independent, and the remaining $n-r$ columns are linear combinations of the first r. We draw it thus:

$$\left(\begin{array}{c|c}\alpha & \beta\\ \hline \beta^* & \gamma\end{array}\right).$$

Then the top left $r\times r$ matrix α is an arbitrary Hermitian matrix and has r^2 degrees of freedom. Each of the remaining $n-r$ columns of length r, making up β, needs r complex coefficients to specify its linear dependence on the first r, so there are $2r(n-r)$ real degrees of freedom in β, making a total of

$$r^2+2r(n-r)=r(2n-r) \tag{2}$$

degrees of freedom altogether. When α and β are specified, so also is the bottom right $(n-r)\times(n-r)$ matrix γ, since the columns of γ must be the same linear combinations of β^* as the columns of β are of α. One can easily verify that γ, so computed, is Hermitian. To obtain the set of all Hermitian $n\times n$ matrices of rank r we must augment the above matrices by matrices whose first r columns are linearly dependent but which have r independent columns altogether. This evidently does not increase the dimension of the set.

A more elegant proof of (2) begins with the observation that a Hermitian operator of rank r on $\mathscr{H}$ has a null space of complex dimension $n-r$. Now the real dimension of the space $\mathscr{V}$ of these $(n-r)$-complex-dimensional subspaces of $\mathscr{H}$ is the dimension of the group $U(n)/(U(n-r)\otimes U(r))$, which is

$$n^2-(n-r)^2-r^2=2r(n-r)$$

since dimension $U(n)=n^2$. Having selected an element $V\in\mathscr{V}$ to be kernel, our operator must be just a Hermitian operator on the orthogonal complement $V^{\perp}$, and so has dimension r^2, giving the same total dimension as before. The dimension of the density operators of rank r on $\mathscr{H}$ is one less than this, because of the trace condition, and so is

$$r(2n-r)-1. \tag{3}$$

5. States of system of spin-$\frac{1}{2}$

In this case, $n=2$ so the convex set of states has two strata, of ranks 1 and 2, and, by equation (3), dimensions 2 and 3 respectively.

In an orthonormal basis of $\mathscr{H}$ the density matrices have the form

$$\omega=\begin{pmatrix} a & h_{\mathrm{R}}-\mathrm{i}h_{\mathrm{I}} \\ h_{\mathrm{R}}+\mathrm{i}h_{\mathrm{I}} & b \end{pmatrix} \tag{4}$$

where the positivity and trace conditions give

$$0\leqslant a\leqslant 1, \qquad 0\leqslant b\leqslant 1, \qquad a+b=1 \tag{5}$$

$$h_{\mathrm{R}}^2+h_{\mathrm{I}}^2\leqslant ab. \tag{6}$$

The pure state which corresponds to the spinor

$$\begin{pmatrix}\alpha\\ \beta\end{pmatrix}, \qquad \alpha,\beta\in\mathbb{C}, \qquad |\alpha|^2+|\beta|^2=1$$

has density matrix

$$\begin{pmatrix} |\alpha|^2 & \bar{\alpha}\beta \\ \bar{\beta}\alpha & |\beta|^2 \end{pmatrix}. \tag{7}$$

We wish to exhibit geometrically the convex set of matrices (4) with the set (7) as the extremal points.

The natural Euclidean space to work in is the 4-dimensional space $(h_{\mathrm{R}}, h_{\mathrm{I}}, a, b)$. Conditions (5) restrict (a, b) to the positive piece of the hyperplane $a+b=1$. We do not lose geometrical understanding if we eliminate b by setting $b=1-a$ in the inequality (6), i.e., we restrict our vision to this 3-dimensional hyperplane and forget its embedding space. The inequality (6) then gives

$$(a-\tfrac{1}{2})+h_{\mathrm{R}}^2+h_{\mathrm{I}}^2\leqslant\tfrac{1}{4} \tag{8}$$

so that the points $(h_{\mathrm{R}}, h_{\mathrm{I}}, a)$ lie inside or on the ball centre $(0, 0, \frac{1}{2})$, radius $\frac{1}{2}$ in Cartesian 3-space. Each point of this ball gives a density matrix. The pure-state density matrix (7) has point $(\mathrm{Re}\,\bar{\alpha}\beta, \mathrm{Im}\,\bar{\alpha}\beta, |\alpha|^2)$ which saturates the inequality (8) and so lies on the surface of the ball.

The points of the surface are in (1, 1) correspondence with the unit rays in $\mathbb{C}^2$. (This mapping from the 3-dimensional sphere S^3 of unit spinors in $\mathbb{C}^2$ to the sphere S^2 in R^3 is known as the Hopf fibration (Spanier 1966), $S^3/S^1=S^2$. The quotient S^1 arises from the invariance of the state (7) under the circle group S^1 of phase transformations $\mathrm{e}^{\mathrm{i}\lambda}$ of the spinor.)

In the spin-$\frac{1}{2}$ case we have therefore a good geometrical picture of the mixed states sitting inside the pure states; the mixed states are the points inside the ball and the pure states are the points on the surface (figure 1). The mixed states have rank 2. The decomposition of a mixed state, point ω, as a convex sum of two pure states ψ_1 and ψ_2 is given geometrically by drawing a straight line through ω; ψ_1 and ψ_2 are its intersections with the sphere. Evidently this may be done in a two-parameter family of ways. The points of the ball are immediately related to the expectation values of the observables J_x, J_y, J_z. Suppose the basis of $\mathscr{H}$ is the eigenbasis of J_z, $|\frac{1}{2}\rangle$ and $|-\frac{1}{2}\rangle$. In this basis,

$$\boldsymbol{J}=(J_x, J_y, J_z)=\frac{1}{2}\left(\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}, \begin{pmatrix}0 & -\mathrm{i}\\ \mathrm{i} & 0\end{pmatrix}, \begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}\right).$$

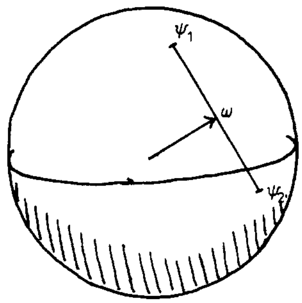

Figure 1. States of a spin-$\frac{1}{2}$ system.

Thus we have, with ω given by (4),

$$\langle J_x \rangle = \mathrm{Tr}(\omega J_x) = h_{\mathrm{R}}, \qquad \langle J_y \rangle = h_{\mathrm{I}}, \qquad \langle J_z \rangle = \tfrac{1}{2}(a-b) = a - \tfrac{1}{2}.$$

Hence we may identify the position vectors $(h_{\mathrm{R}}, h_{\mathrm{I}}, a-\frac{1}{2})$ of the point ω of the ball relative to its centre $(0, 0, \frac{1}{2})$ with the expectation value $\langle \boldsymbol{J} \rangle$ of the angular momentum in the corresponding state. Several properties of spin-$\frac{1}{2}$ states are now evident visually. For example, if $\langle J_x \rangle^2 + \langle J_y \rangle^2 + \langle J_z \rangle^2 = \frac{1}{4}$ then the state is pure. Only one state is completely unpolarized, $\langle \boldsymbol{J} \rangle = 0$. The entire information possessed by a spin-$\frac{1}{2}$ state is embodied in its three expectation values $\langle \boldsymbol{J} \rangle$. In the happy phrase of Park and Band (1971) the set $\{J_x, J_y, J_z\}$ constitutes a quorum of observables.

6. States of system of spin-1

In the notation of § 4, $\mathscr{H} = \mathbb{C}^3$, $n = 3$, so the convex set of states has 3 strata, ranks 1, 2, 3 with dimensions 4, 7, 8. Typically

$$\omega = \begin{pmatrix} a & \bar{h} & g \\ h & b & \bar{f} \\ \bar{g} & f & c \end{pmatrix} \qquad a, b, c \in \mathbb{R}, f, g, h \in \mathbb{C} \tag{9}$$

with a trace condition

$$a + b + c = 1 \tag{10}$$

and the positivity conditions (for example, Frazer *et al* 1957)

$$a \geqslant 0, \qquad b \geqslant 0, \qquad c \geqslant 0 \tag{11}$$

$$|f|^2 \leqslant bc, \qquad |g|^2 \leqslant ca, \qquad |h|^2 \leqslant ab \tag{12}$$

$$\det \omega \equiv abc + 2\,\mathrm{Re}(fgh) - (a|f|^2 + b|g|^2 + c|h|^2) \geqslant 0. \tag{13}$$

The matrices ω of rank 3 (for which $\det \omega > 0$) form a convex region of R^8. We shall investigate the shape of this region and see how the 4-dimensional subregion of pure states of rank 1

$$\begin{pmatrix} |\alpha|^2 & \bar{\alpha}\beta & \bar{\alpha}\gamma \\ \bar{\beta}\alpha & |\beta|^2 & \bar{\beta}\gamma \\ \bar{\gamma}\alpha & \bar{\gamma}\beta & |\gamma|^2 \end{pmatrix}, \qquad |\alpha|^2 + |\beta|^2 + |\gamma|^2 = 1,$$

(for which (12) and (13) are equalities) sits in the 7-dimensional boundary of mixed states of rank 2 (for which $\det\omega = 0$).

Regions of space of dimension greater than 4 are hard to visualize. One can to some extent imagine a 4-dimensional region as a family of 3-dimensional slices. We have a better chance with convex regions than with others since they can have no subtlety of connectivity and any plane slice of the region is again convex. We shall examine the 8-dimensional region step by step.

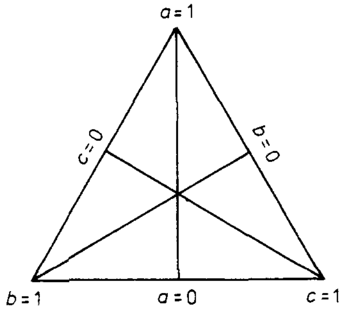

Figure 2. The triangle Δ.

We start with the allowed values of a, b, c. The trace condition (10) and condition (11) restrict a, b, c to the triangle Δ of the plane $a+b+c=1$ which lies in the positive octant, figure 2. Each point in Δ corresponds to an allowed set of values (a, b, c). Over each interior point (a, b, c) of Δ there is a convex 6-dimensional region of allowed values $(f_R, f_I, g_R, g_I, h_R, h_I)$. It follows from the inequalities (12) that this region collapses to the point $f=g=h=0$ at the vertices of Δ, to the 2-dimensional disc $|f|^2 \leqslant bc$, $g=h=0$ on the edge $a=0$ of Δ, and to corresponding discs on the other two edges of Δ. Suppose now that (a, b, c) is an interior point of Δ. We wish to describe the allowed region of (f, g, h) space at this point, given by (12) and (13). It is convenient to suppress the dependence on a, b and c by scaling the variables f, g, h. We set

$$f=\sqrt{bc}F, \qquad g=\sqrt{ca}G, \qquad h=\sqrt{ab}H. \tag{14}$$

The inequalities (12) and (13) become

$$\begin{gathered} |F|\leqslant 1, \qquad |G|\leqslant 1, \qquad |H|\leqslant 1 \\ |F|^2+|G|^2+|H|^2-2\,\mathrm{Re}(FGH)\leqslant 1. \end{gathered} \tag{15}$$

The region of (F, G, H) space determined by these inequalities is evidently symmetrical in F, G, H. Let us fix F in its disc $|F|\leqslant 1$ and compute the 4-dimensional allowed region for (G_R, G_I, H_R, H_I). In (14) the phase $\arg F = \chi_F$ appears only in the term $2\,\mathrm{Re}(FGH)$ and so only appears summed with the phases of G and H. Hence the regions in the (G, H) space for all values of χ_F and constant $|F|$ are identical in *shape*, though they will have different orientations with respect to the axes. To find this shape we shall take F real for simplicity. Condition (15) then gives

$$1-F^2 \geqslant G_R^2+G_I^2+H_R^2+H_I^2-2F(G_RH_R-G_IH_I).$$

By the standard methods of coordinate geometry (e.g. Leithold 1972) we may rotate the (G_R, H_R) axes and the (G_I, H_I) axes through $\pi/4$ to find that the allowed values of

(G, H) lie inside a 4-dimensional spheroid whose principal axes have lengths A_+, A_+, A_-, A_- given by

$$A_\pm = (1 \pm F)^{1/2}.$$

As $|F|$ approaches its limiting value 1, we see that this 4-spheroid thins out to a 2-dimensional disc. The same result holds if F is complex, which henceforth we shall take it to be. This behaviour of the shape may also be found directly from condition (15) with $F = e^{i\chi_F}$, which gives

$$|G\,e^{i\chi_F} - \bar{H}|^2 \leqslant 0$$

i.e.

$$G\,e^{i\chi_F} = \bar{H}. \tag{16}$$

This restricts G and H in (G, H) 4-space to a 2-plane through the origin. Then the condition

$$|G| \leqslant 1$$

or equivalently, by (16)

$$|H| \leqslant 1$$

gives the disc. It follows from (16) that when $|G| = 1$ so also $|H| = 1$ so that on the edges of this disc we may write

$$F = e^{i\chi_F}, \qquad G = e^{i\chi_G}, \qquad H = e^{i\chi_H}$$

$$f = \sqrt{bc}\,e^{i\chi_F}, \qquad g = \sqrt{ca}\,e^{i\chi_G}, \qquad h = \sqrt{ab}\,e^{i\chi_H}$$

where by (16)

$$\chi_F + \chi_G + \chi_H = 0.$$

Thus setting $\alpha = \sqrt{a}$, $\beta = \sqrt{b}\,e^{-i\chi_h}$, $\gamma = \sqrt{c}\,e^{i\chi_g}$ (or any constant phase times these) we see

$$\begin{pmatrix} a & \bar{h} & g \\ h & b & \bar{f} \\ \bar{g} & f & c \end{pmatrix} = \begin{pmatrix} |\alpha|^2 & \bar{\alpha}\beta & \bar{\alpha}\gamma \\ \bar{\beta}\alpha & |\beta|^2 & \bar{\beta}\gamma \\ \bar{\gamma}\alpha & \bar{\gamma}\beta & |\gamma|^2 \end{pmatrix}.$$

Thus the points on this disc are in (1, 1) correspondence with the unit rays of $\mathcal{H}$. We see from the symmetric nature of the result that if we had first fixed $g = \sqrt{ca}\,e^{i\chi_G}$ or $h = \sqrt{ab}\,e^{i\chi_H}$ and computed the allowed values of h, f or of f, g respectively, we should obtain again the *same* set of extreme points, and not new sets. In topological terms this set is $S^5/S^1 = P^2\mathbb{C}$, the complex projective plane.

Inside the region, we have $\det \omega > 0$ by inequality (13) so the rank of ω is 3. Every point in this region can be written as a convex combination of 3 pure points, and of not less than 3. On the boundary, $\det \omega = 0$, the rank is 1 or 2. Thus, inside the (g, h) 4-ellipsoids the rank is 3. On them, the rank is 2. On the extremal discs, the states are pure and the rank is 1. Of course, since f, g and h appear symmetrically in the problem, to each cross section we have obtained by fixing f there will be symmetrical results for fixing g or h.

7. Real section

The convex set described in § 6 was 8-dimensional and hard to visualize. It was the set of positive Hermitian 3×3 complex matrices of unit trace. We compute here the real section of this set, the projection onto the hyperplane $f_I = g_I = h_I = 0$. This is the set of positive symmetric real matrices of unit trace, and may be viewed also as the set of states of a system whose algebra of observables is the 3×3 real matrix algebra. The pure states are the unit rays of R^3; they form the 2-dimensional space $S^2/Z_2 = P^2R$. The mixed states of rank 3 form a 5-dimensional set; its 4-dimensional boundary consists almost entirely of rank 2 states but contains the pure states as a 2-dimensional subset. We now investigate how these strata fit together. The general density matrix is again (9) where a, b, c, f, g, h obey (10)–(13) but now f, g and h are real.

The conditions (10) and (11) again restrict (a, b, c) to the triangle Δ of figure 2. Over each point (a, b, c) in Δ the allowed points (f, g, h) form a 3-dimensional region determined by the inequalities

$$f^2 \leqslant bc, \qquad g^2 \leqslant ca, \qquad h^2 \leqslant ab$$
$$abc + 2fgh - (af^2 + bg^2 + ch^2) \geqslant 0,$$

which become

$$\begin{aligned} &-1 \leqslant F, G, H \leqslant 1 \\ &F^2 + G^2 + H^2 - 2FGH \leqslant 1 \end{aligned} \tag{17}$$

upon making the substitution (14). Consider the plane sections F equals a constant of the boundary of this region. If $F = 0$, the section is the circle $G^2 + H^2 = 1$. If $F = 1$, it is the segment of the line $G = H$ from $(-1, -1)$ to $(1, 1)$, and if $F = -1$ it is the segment of the line $G = -H$ from $(1, -1)$ to $(-1, 1)$. For intermediate values of F the section is an ellipse. The shape thus contains the vertices $(-1, 1, -1)$, $(-1, -1, 1)$, $(1, -1, -1)$, $(1, 1, 1)$ of a tetrahedron and its edges. Further investigation shows that along these edges, the shape touches the faces of the cube whose corners are $(\pm 1, \pm 1, \pm 1)$. So the shape is like that of an overfilled tetrapak carton, drawn in figure 3. If we now rescale back to the variables f, g, h then the cube distorts to a rectangular block, and it degenerates to a line segment on the edges of Δ. The pure states are at the four corners of the tetrapak. We observed that the pure states form a 2-sphere S^2 with diametrical points identified by the reflection group Z_2. Such a space has 4 sectors (the octants of S^2

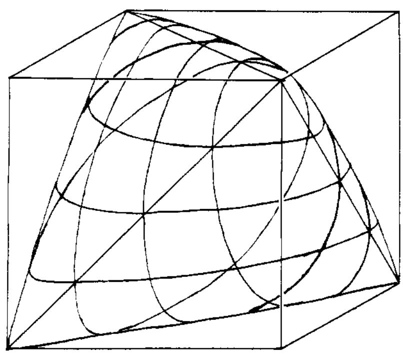

Figure 3. The region determined by conditions (17).

with opposite points identified) and each sector maps onto the triangle Δ to provide, at each interior point of Δ, one of the four pure states. The identifications at the edges of the sectors ensure that there are 2 pure states at each interior point of the edge of Δ and one pure state at each vertex of Δ.

Acknowledgments

I thank J Borwein, E Ihrig, D Kiang and A Niegawa for helpful comments and the Izaak Walton Killam Foundation for a Fellowship at the very hospitable Department of Physics, Dalhousie University.

References

Eggleston H G 1969 *Convexity* (Cambridge: Cambridge University Press)
Frazer R A, Duncan W J and Collar A R 1957 *Elementary Matrices* (Cambridge: Cambridge University Press) p 31
Leithold L 1972 *The Calculus with Analytic Geometry* (New York: Harper and Row) chap. 12
Park J L and Band W 1971 *Found. Phys.* **1** 211–26
Segal I E 1947 *Ann. Math., NY* **48** 930–48
Spanier E 1966 *Algebraic Topology* (New York: McGraw-Hill) p 91