Part I

Basic Mathematics

1

Basic Mathematical Background: Introduction

In this chapter we introduce the mathematical definitions and concepts that are basic to group theory and to the classification of symmetry properties [2].

1.1 Definition of a Group

A collection of elements $A, B, C, \ldots$ form a group when the following four conditions are satisfied:

1. The product of any two elements of the group is itself an element of the group. For example, relations of the type $AB = C$ are valid for all members of the group.
2. The associative law is valid – i.e., $(AB)C = A(BC)$.
3. There exists a unit element E (also called the identity element) such that the product of E with any group element leaves that element unchanged $AE = EA = A$.
4. For every element A there exists an inverse element A^{-1} such that $A^{-1}A = AA^{-1} = E$.

In general, the elements of a group will not commute, i.e., $AB \neq BA$. But if all elements of a group commute, the group is then called an *Abelian* group.

1.2 Simple Example of a Group

As a simple example of a group, consider the permutation group for three numbers, $P(3)$. Equation (1.1) lists the $3! = 6$ possible permutations that can be carried out; the top row denotes the initial arrangement of the three numbers and the bottom row denotes the final arrangement. Each permutation is an element of $P(3)$.

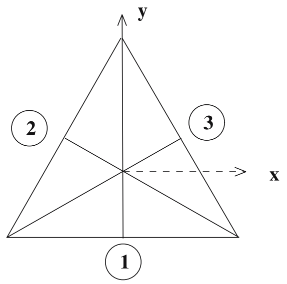

Fig. 1.1. The symmetry operations on an equilateral triangle are the rotations by $\pm 2\pi/3$ about the origin and the rotations by π about the three twofold axes. Here the axes or points of the equilateral triangle are denoted by numbers in *circles*

$$
\begin{aligned}
E &= \begin{pmatrix} 1\,2\,3 \\ 1\,2\,3 \end{pmatrix} \quad A = \begin{pmatrix} 1\,2\,3 \\ 1\,3\,2 \end{pmatrix} \quad B = \begin{pmatrix} 1\,2\,3 \\ 3\,2\,1 \end{pmatrix} \\
C &= \begin{pmatrix} 1\,2\,3 \\ 2\,1\,3 \end{pmatrix} \quad D = \begin{pmatrix} 1\,2\,3 \\ 3\,1\,2 \end{pmatrix} \quad F = \begin{pmatrix} 1\,2\,3 \\ 2\,3\,1 \end{pmatrix} .
\end{aligned} \tag{1.1}
$$

We can also think of the elements in (1.1) in terms of the three points of an equilateral triangle (see Fig. 1.1). Again, the top row denotes the initial state and the bottom row denotes the final position of each number. For example, in symmetry operation D, 1 moves to position 2, and 2 moves to position 3, while 3 moves to position 1, which represents a clockwise rotation of $2\pi/3$ (see caption to Fig. 1.1). As the effect of the six distinct symmetry operations that can be performed on these three points (see caption to Fig. 1.1). We can call each symmetry operation an *element* of the group. The P(3) group is, therefore, identical with the group for the symmetry operations on a equilateral triangle shown in Fig. 1.1. Similarly, F is a counter-clockwise rotation of $2\pi/3$, so that the numbers inside the circles in Fig. 1.1 move exactly as defined by Eq. 1.1.

It is convenient to classify the products of group elements. We write these products using a *multiplication table*. In Table 1.1 a multiplication table is written out for the symmetry operations on an equilateral triangle or equivalently for the permutation group of three elements. It can easily be shown that the symmetry operations given in (1.1) satisfy the four conditions in Sect. 1.1 and therefore form a group. We illustrate the use of the notation in Table 1.1 by verifying the *associative law* $(AB)C = A(BC)$ for a few elements:

$$
\begin{aligned}
(AB)C &= DC = B \\
A(BC) &= AD = B .
\end{aligned} \tag{1.2}
$$

Each element of the permutation group $P(3)$ has a one-to-one correspondence to the symmetry operations of an equilateral triangle and we therefore say that these two groups are *isomorphic* to each other. We furthermore can

Table 1.1. Multiplication[a] table for permutation group of three elements; $P(3)$

	E	A	B	C	D	F
E	E	A	B	C	D	F
A	A	E	D	F	B	C
B	B	F	E	D	C	A
C	C	D	F	E	A	B
D	D	C	A	B	F	E
F	F	B	C	A	E	D

[a] $AD = B$ defines use of multiplication table

use identical group theoretical procedures in dealing with physical problems associated with either of these groups, even though the two groups arise from totally different physical situations. It is this generality that makes group theory so useful as a general way to classify symmetry operations arising in physical problems.

Often, when we deal with symmetry operations in a crystal, the geometrical visualization of repeated operations becomes difficult. Group theory is designed to help with this problem. Suppose that the symmetry operations in practical problems are elements of a group; this is generally the case. Then if we can associate each element with a matrix that obeys the same multiplication table as the elements themselves, that is, if the elements obey $AB = D$, then the matrices representing the elements must obey

$$M(A)\,M(B) = M(D)\,. \tag{1.3}$$

If this relation is satisfied, then we can carry out all geometrical operations analytically in terms of arithmetic operations on matrices, which are usually easier to perform. The one-to-one identification of a generalized symmetry operation with a matrix is the basic idea of a *representation* and why group theory plays such an important role in the solution of practical problems.

A set of matrices that satisfy the multiplication table (Table 1.1) for the group $P(3)$ are:

$$E = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad A = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix} \quad B = \begin{pmatrix} \frac{1}{2} & -\frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}$$

$$C = \begin{pmatrix} \frac{1}{2} & \frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix} \quad D = \begin{pmatrix} -\frac{1}{2} & \frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix} \quad F = \begin{pmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}\,. \tag{1.4}$$

We note that the matrix corresponding to the identity operation E is always a unit matrix. The matrices in (1.4) constitute a matrix representation of the group that is isomorphic to $P(3)$ and to the symmetry operations on an equilateral triangle. The A matrix represents a rotation by $\pm\pi$ about the y axis, while the B and C matrices, respectively, represent rotations by $\pm\pi$ about axes 2 and 3 in Fig. 1.1. D and F, respectively, represent rotation of $-2\pi/3$ and $+2\pi/3$ around the center of the triangle.

1.3 Basic Definitions

Definition 1. *The order of a group ≡ the number of elements in the group. We will be mainly concerned with finite groups. As an example,* $P(3)$ *is of order 6.*

Definition 2. *A subgroup ≡ a collection of elements within a group that by themselves form a group.*

Examples of subgroups in $P(3)$:

$$\begin{array}{lll} E & (E,A) & (E,D,F) \\ & (E,B) & \\ & (E,C) & \end{array}$$

Theorem. *If in a finite group, an element* X *is multiplied by itself enough times (n), the identity* $X^n = E$ *is eventually recovered.*

Proof. If the group is finite, and any arbitrary element is multiplied by itself repeatedly, the product will eventually give rise to a repetition. For example, for $P(3)$ which has six elements, seven multiplications must give a repetition. Let Y represent such a repetition:

$$Y = X^p = X^q \ , \quad \text{where} \quad p > q \ . \tag{1.5}$$

Then let $p = q + n$ so that

$$X^p = X^{q+n} = X^q X^n = X^q = X^q E \ , \tag{1.6}$$

from which it follows that

$$X^n = E \ . \tag{1.7}$$

□

Definition 3. *The order of an element ≡ the smallest value of* n *in the relation* $X^n = E$.

We illustrate the order of an element using $P(3)$ where:

- E is of order 1,
- A, B, C are of order 2,
- D, F are of order 3.

Definition 4. *The period of an element* $X \equiv$ *collection of elements* E, X, X^2, $\ldots, X^{n-1}$, *where* n *is the order of the element. The period forms an Abelian subgroup.*

Some examples of periods based on the group $P(3)$ *are*

$$\begin{aligned}&E, A\\&E, B\\&E, C\\&E, D, F = E, D, D^2 \,.\end{aligned} \tag{1.8}$$

1.4 Rearrangement Theorem

The rearrangement theorem is fundamental and basic to many theorems to be proven subsequently.

Rearrangement Theorem. *If* $E, A_1, A_2, \ldots, A_h$ *are the elements of a group, and if* A_k *is an arbitrary group element, then the assembly of elements*

$$A_kE, A_kA_1, \ldots, A_kA_h \tag{1.9}$$

contains each element of the group once and only once.

Proof. 1. We show first that every element is contained.
Let X be an arbitrary element. If the elements form a group there will be an element $A_r = A_k^{-1}X$. Then $A_kA_r = A_kA_k^{-1}X = X$. Thus we can always find X after multiplication of the appropriate group elements.

2. We now show that X occurs only once. Suppose that X appears twice in the assembly $A_kE, A_kA_1, \ldots, A_kA_h$, say $X = A_kA_r = A_kA_s$. Then by multiplying on the left by A_k^{-1} we get $A_r = A_s$, which implies that two elements in the original group are identical, contrary to the original listing of the group elements.

Because of the rearrangement theorem, every row and column of a multiplication table contains each element once and only once. □

1.5 Cosets

In this section we will introduce the concept of cosets. The importance of cosets will be clear when introducing the factor group (Sect. 1.7). The cosets are the elements of a factor group, and the factor group is important for working with space groups (see Chap. 9).

Definition 5. *If* $\mathcal{B}$ *is a subgroup of the group* G, *and* X *is an element of* G, *then the assembly* $EX, B_1X, B_2X, \ldots, B_gX$ *is the right coset of* $\mathcal{B}$, *where* $\mathcal{B}$ *consists of* $E, B_1, B_2, \ldots, B_g$.

A coset need not be a subgroup. A coset will itself be a subgroup $\mathcal{B}$ *if* X *is an element of* $\mathcal{B}$ *(by the rearrangement theorem).*

Theorem. *Two right cosets of given subgroup either contain exactly the same elements, or else have no elements in common.*

Proof. Clearly two right cosets either contain no elements in common or at least one element in common. We show that if there is one element in common, all elements are in common.

Let $\mathcal{B}X$ and $\mathcal{B}Y$ be two right cosets. If $B_kX = B_\ell Y =$ one element that the two cosets have in common, then

$$B_\ell^{-1}B_k = YX^{-1} \tag{1.10}$$

and YX^{-1} is in $\mathcal{B}$, since the product on the left-hand side of (1.10) is in $\mathcal{B}$. And also contained in $\mathcal{B}$ is EYX^{-1}, B_1YX^{-1}, B_2YX^{-1}, ... , B_gYX^{-1}. Furthermore, according to the rearrangement theorem, these elements are, in fact, identical with $\mathcal{B}$ except for possible order of appearance. Therefore the elements of $\mathcal{B}Y$ are identical to the elements of $\mathcal{B}YX^{-1}X$, which are also identical to the elements of $\mathcal{B}X$ so that all elements are in common. □

We now give some examples of cosets using the group $P(3)$. Let $\mathcal{B} = E, A$ be a subgroup. Then the right cosets of $\mathcal{B}$ are

$$\begin{array}{ll} (E,A)E \to E,A & (E,A)C \to C,F \\ (E,A)A \to A,E & (E,A)D \to D,B \\ (E,A)B \to B,D & (E,A)F \to F,C \ , \end{array} \tag{1.11}$$

so that there are three distinct right cosets of (E, A), namely

$$\begin{array}{ll} (E,A) & \text{which is a subgroup} \\ (B,D) & \text{which is not a subgroup} \\ (C,F) & \text{which is not a subgroup.} \end{array}$$

Similarly there are three left cosets of (E, A) obtained by $X(E, A)$:

$$\begin{array}{l} (E,A) \\ (C,D) \\ (B,F)\ . \end{array} \tag{1.12}$$

To multiply two cosets, we multiply constituent elements of each coset in proper order. Such multiplication either yields a coset or joins two cosets. For example:

$$(E,A)(B,D) = (EB,ED,AB,AD) = (B,D,D,B) = (B,D)\ . \tag{1.13}$$

Theorem. *The order of a subgroup is a divisor of the order of the group.*

Proof. If an assembly of all the distinct cosets of a subgroup is formed (n of them), then n multiplied by the number of elements in a coset, $\mathcal{C}$, is exactly the number of elements in the group. Each element must be included since cosets have no elements in common.

For example, for the group $P(3)$, the subgroup (E, A) is of order 2, the subgroup (E, D, F) is of order 3 and both 2 and 3 are divisors of 6, which is the order of $P(3)$. □

1.6 Conjugation and Class

Definition 6. *An element B conjugate to A is by definition $B \equiv XAX^{-1}$, where X is an arbitrary element of the group.*

For example,

$$A = X^{-1}BX = YBY^{-1}\,, \quad \text{where} \quad BX = XA \quad \text{and} \quad AY = YB\,.$$

The elements of an Abelian group are all selfconjugate.

Theorem. *If B is conjugate to A and C is conjugate to B, then C is conjugate to A.*

Proof. By definition of conjugation, we can write

$$\begin{aligned} B &= XAX^{-1} \\ C &= YBY^{-1}\,. \end{aligned}$$

Thus, upon substitution we obtain

$$C = YXAX^{-1}Y^{-1} = YXA(YX)^{-1}\,.$$

□

Definition 7. *A class is the totality of elements which can be obtained from a given group element by conjugation.*

For example in $P(3)$, there are three classes:

1. E;
2. A, B, C;
3. D, F.

Consistent with this class designation is

$$ABA^{-1} = AF = C \tag{1.14}$$

$$DBD^{-1} = DA = C\,. \tag{1.15}$$

Note that each class corresponds to a physically distinct kind of symmetry operation such as rotation of π about equivalent twofold axes, or rotation of $2\pi/3$ about equivalent threefold axes. The identity symmetry element is always in a class by itself. An *Abelian* group has as many classes as elements. The identity element is the only class forming a group, since none of the other classes contain the identity.

Theorem. *All elements of the same class have the same order.*

Proof. The order of an element n is defined by $A^n = E$. An arbitrary conjugate of A is $B = XAX^{-1}$. Then $B^n = (XAX^{-1})(XAX^{-1}) \ldots n$ times gives $XA^nX^{-1} = XEX^{-1} = E$.

Definition 8. *A subgroup $\mathcal{B}$ is* self-conjugate (*or invariant, or normal*) *if $X\mathcal{B}X^{-1}$ is identical with $\mathcal{B}$ for all possible choices of X in the* group.

For example (E, D, F) forms a self-conjugate subgroup of $P(3)$, but (E, A) does not. The subgroups of an Abelian group are self-conjugate subgroups. We will denote self-conjugate subgroups by $\mathcal{N}$. To form a self-conjugate subgroup, it is necessary to include entire classes in this subgroup.

Definition 9. *A group with no self-conjugate subgroups $\equiv$ a simple group.*

Theorem. *The right and left cosets of a self-conjugate subgroup $\mathcal{N}$ are the same.*

Proof. If N_i is an arbitrary element of the subgroup $\mathcal{N}$, then the left coset is found by elements $XN_i = XN_iX^{-1}X = N_jX$, where the right coset is formed by the elements N_jX, where $N_j = XN_kX^{-1}$.

For example in the group $P(3)$, one of the right cosets is $(E, D, F)A = (A, C, B)$ and one of the left cosets is $A(E, D, F) = (A, B, C)$ and both cosets are identical except for the listing of the elements. □

Theorem. *The multiplication of the elements of two right cosets of a self-conjugate subgroup gives another right coset.*

Proof. Let $\mathcal{N}X$ and $\mathcal{N}Y$ be two right cosets. Then multiplication of two right cosets gives

$$\begin{aligned}(\mathcal{N}X)(\mathcal{N}Y) &\Rightarrow N_iXN_\ell Y = N_i(XN_\ell)Y \\ &= N_i(N_mX)Y = (N_iN_m)(XY) \Rightarrow \mathcal{N}(XY)\end{aligned} \tag{1.16}$$

and $\mathcal{N}(XY)$ denotes a right coset. □

The elements in one right coset of $P(3)$ are $(E, D, F)A = (A, C, B)$ while $(E, D, F)D = (D, F, E)$ is another right coset. The product $(A, C, B)(D, F, E)$ is (A, B, C) which is a right coset. Also the product of the two right cosets $(A, B, C)(A, B, C)$ is (D, F, E) which is a right coset.

1.7 Factor Groups

Definition 10. *The* factor group *(or quotient group) is constructed with respect to a self-conjugate subgroup as the collection of cosets of the self-conjugate subgroup, each coset being considered an element of the factor group. The factor group satisfies the four rules of Sect. 1.1 and is therefore a group:*

1. Multiplication – $(\mathcal{N}X)(\mathcal{N}Y) = \mathcal{N}XY$.
2. Associative law – holds because it holds for the elements.
3. Identity – $E\mathcal{N}$, where E is the coset that contains the identity element. $\mathcal{N}$ is sometimes called a *normal divisor*.
4. Inverse – $(X\mathcal{N})(X^{-1}\mathcal{N}) = (\mathcal{N}X)(X^{-1}\mathcal{N}) = \mathcal{N}^2 = E\mathcal{N}$.

Definition 11. *The* index *of a subgroup* $\equiv$ *total number of cosets* = (*order of group*)/(*order of subgroup*).

The order of the factor group is the index of the self-conjugate subgroup.

In Sect. 1.6 we saw that (E, D, F) forms a self-conjugate subgroup, $\mathcal{N}$. The only other coset of this subgroup $\mathcal{N}$ is (A, B, C), so that the order of this factor group = 2. Let $(A, B, C) = \mathcal{A}$ and $(E, D, F) = \mathcal{E}$ be the two elements of the factor group. Then the multiplication table for this factor group is

	$\mathcal{E}$	$\mathcal{A}$
$\mathcal{E}$	$\mathcal{E}$	$\mathcal{A}$
$\mathcal{A}$	$\mathcal{A}$	$\mathcal{E}$

$\mathcal{E}$ is the identity element of this factor group. $\mathcal{E}$ and $\mathcal{A}$ are their own inverses. From this illustration you can see how the four group properties (see Sect. 1.1) apply to the factor group by taking an element in each coset, carrying out the multiplication of the elements and finding the coset of the resulting element. Note that this multiplication table is also the multiplication table for the group for the permutation of two objects $P(2)$, i.e., this factor group maps one-on-one to the group $P(2)$. This analogy between the factor group and $P(2)$ gives insights into what the factor group is about.

1.8 Group Theory and Quantum Mechanics

We have now learned enough to start making connection of group theory to physical problems. In such problems we typically have a system described by a Hamiltonian which may be very complicated. Symmetry often allows us to make certain simplifications, without knowing the detailed Hamiltonian. To make a connection between group theory and quantum mechanics, we consider the group of symmetry operators $\hat{P}_R$ which leave the Hamiltonian invariant. These operators $\hat{P}_R$ are symmetry operations of the system and the $\hat{P}_R$ operators commute with the Hamiltonian. The operators $\hat{P}_R$ are said to form *the group of the Schrödinger equation.* If $\mathcal{H}$ and $\hat{P}_R$ commute, and if $\hat{P}_R$ is a Hermitian operator, then $\mathcal{H}$ and $\hat{P}_R$ can be simultaneously diagonalized.

We now show that these operators form a group. The identity element clearly exists (leaving the system unchanged). Each symmetry operator $\hat{P}_R$ has an inverse $\hat{P}_R^{-1}$ to undo the operation $\hat{P}_R$ and from physical considerations the element $\hat{P}_R^{-1}$ is also in the group. The product of two operators of the group is still an operator of the group, since we can consider these separately as acting on the Hamiltonian. The associative law clearly holds. Thus the requirements for forming a group are satisfied.

Whether the operators $\hat{P}_R$ be rotations, reflections, translations, or permutations, these symmetry operations do not alter the Hamiltonian or its eigenvalues. If $\mathcal{H}\psi_n = E_n\psi_n$ is a solution to Schrödinger's equation and $\mathcal{H}$ and $\hat{P}_R$ commute, then

$$\hat{P}_R\mathcal{H}\psi_n = \hat{P}_R E_n\psi_n = \mathcal{H}(\hat{P}_R\psi_n) = E_n(\hat{P}_R\psi_n)\ . \tag{1.17}$$

Thus $\hat{P}_R\psi_n$ is as good an eigenfunction of $\mathcal{H}$ as ψ_n itself. Furthermore, both ψ_n and $\hat{P}_R\psi_n$ correspond to the *same* eigenvalue E_n. Thus, starting with a particular eigenfunction, we can generate all other eigenfunctions of the same degenerate set (same energy) by applying all the symmetry operations that commute with the Hamiltonian (or leave it invariant). Similarly, if we consider the product of two symmetry operators, we again generate an eigenfunction of the Hamiltonian $\mathcal{H}$

$$\begin{aligned} &\hat{P}_R\hat{P}_S\mathcal{H} = \mathcal{H}\hat{P}_R\hat{P}_S \\ &\hat{P}_R\hat{P}_S\mathcal{H}\psi_n = \hat{P}_R\hat{P}_S E_n\psi_n = E_n(\hat{P}_R\hat{P}_S\psi_n) = \mathcal{H}(\hat{P}_R\hat{P}_S\psi_n)\ , \end{aligned} \tag{1.18}$$

in which $\hat{P}_R\hat{P}_S\psi_n$ is also an eigenfunction of $\mathcal{H}$. We also note that the action of $\hat{P}_R$ on an arbitrary vector consisting of ℓ eigenfunctions, yields a $\ell \times \ell$ matrix representation of $\hat{P}_R$ that is in block diagonal form. The representation of physical systems, or equivalently their symmetry groups, in the form of matrices is the subject of the next chapter.

Selected Problems

1.1. (a) Show that the trace of an arbitrary square matrix X is invariant under a similarity (or equivalence) transformation UXU^{-1}.

(b) Given a set of matrices that represent the group G, denoted by $D(R)$ (for all R in G), show that the matrices obtainable by a similarity transformation $UD(R)U^{-1}$ also are a representation of G.

1.2. (a) Show that the operations of $P(3)$ in (1.1) form a group, referring to the rules in Sect. 1.1.

(b) Multiply the two left cosets of subgroup (E, A): (B, F) and (C, D), referring to Sect. 1.5. Is the result another coset?

(c) Prove that in order to form a normal (self-conjugate) subgroup, it is necessary to include only entire classes in this subgroup. What is the physical consequence of this result?
(d) Demonstrate that the normal subgroup of $P(3)$ includes entire classes.

1.3. (a) What are the symmetry operations for the molecule AB_4, where the B atoms lie at the corners of a square and the A atom is at the center and is not coplanar with the B atoms.
(b) Find the multiplication table.
(c) List the subgroups. Which subgroups are self-conjugate?
(d) List the classes.
(e) Find the multiplication table for the factor group for the self-conjugate subgroup(s) of (c).

1.4. The group defined by the permutations of four objects, $P(4)$, is isomorphic (has a one-to-one correspondence) with the group of symmetry operations of a regular tetrahedron (T_d). The symmetry operations of this group are sufficiently complex so that the power of group theoretical methods can be appreciated. For notational convenience, the elements of this group are listed below.

$$
\begin{array}{llll}
e = (1234) & g = (3124) & m = (1423) & s = (4213) \\
a = (1243) & h = (3142) & n = (1432) & t = (4231) \\
b = (2134) & i = (2314) & o = (4123) & u = (3412) \\
c = (2143) & j = (2341) & p = (4132) & v = (3421) \\
d = (1324) & k = (3214) & q = (2413) & w = (4312) \\
f = (1342) & l = (3241) & r = (2431) & y = (4321)\,.
\end{array}
$$

Here we have used a shorthand notation to denote the elements: for example $j = (2341)$ denotes

$$
\begin{pmatrix} 1\,2\,3\,4 \\ 2\,3\,4\,1 \end{pmatrix} ,
$$

that is, the permutation which takes objects in the order 1234 and leaves them in the order 2341:

(a) What is the product vw? wv?
(b) List the subgroups of this group which correspond to the symmetry operations on an equilateral triangle.
(c) List the right and left cosets of the subgroup (e, a, k, l, s, t).
(d) List all the symmetry classes for $P(4)$, and relate them to symmetry operations on a regular tetrahedron.
(e) Find the factor group and multiplication table formed from the self-conjugate subgroup (e, c, u, y). Is this factor group isomorphic to $P(3)$?