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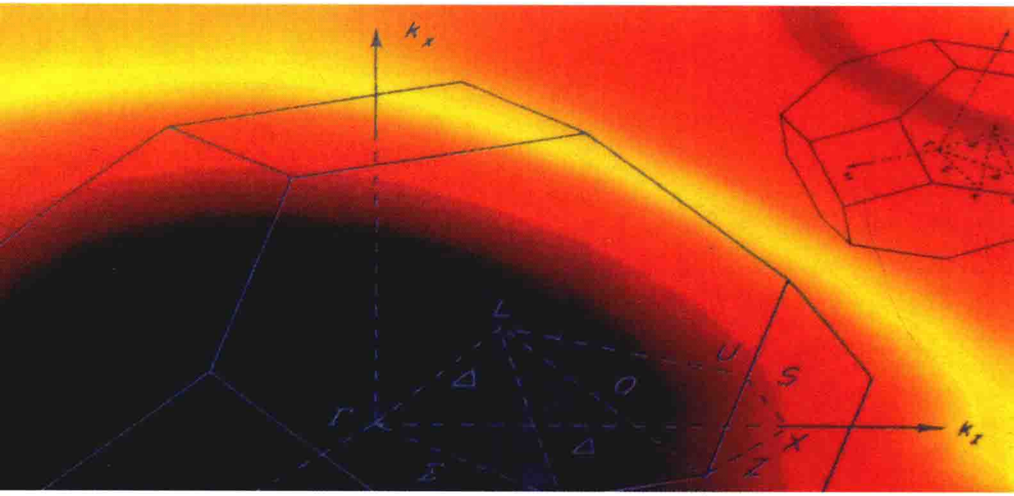
GROUP THEORY IN PHYSICS



AN INTRODUCTION

J. F. CORNWELL

物理学中的群论导论

Elsevier (Singapore) Pte Ltd.

世界图书出版公司
www.wpcbj.com.cn

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群论是处理经典物理和量子物理诸多问题的必备工具。本书详细介绍了群的结构、群表示论、李群、半单李群、转动群、固体空间群、李群与李代数等知识。本书在照顾了非数学、非理论物理专业研究生的阅读习惯的基础上，依然保持了严谨的数学风格，适用于从事理论物理、固体物理和量子化学等领域的科研教学人员和研究生。对于许多已经从不同方向上不同层次地接触过群论又想系统学习群论的读者，本书也是一本优秀的入门参考书。

ISBN 7-5062-7304-7
9 787506 273046 >

ISBN 7-5062-7304-7/O·566
WB7304　　定价：58.00元

Group Theory in Physics

An Introduction

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ACADEMIC PRESS
Harcourt Brace & Company, Publishers
San Diego London Boston New York
Sydney Tokyo Toronto

图书在版编目（C I P）数据

物理学中的群论导论/（美）康威尔（Cornwell,J.F.）
著. 一北京：世界图书出版公司北京公司，2006.12
书名原文：Group Theory In Physics：An Introduc tion
ISBN 7-5062-7304-7

Ⅰ.物… Ⅱ.康… Ⅲ. 群论－应用－物理学－教
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中国版本图书馆CIP数据核字（2006）第139572号

书　　名：Group Theory in Physics: an Introduction
作　　者：John F. Cornwell
中 译 名：物理学中的群论导论
责任编辑：高　蓉

出 版 者：世界图书出版公司北京公司
印 刷 者：北京世图印刷厂
发　　行：世界图书出版公司北京公司（北京朝内大街 137 号　100010）
联系电话：010-64015659, 64038347
电子信箱：kjsk@vip.si [redacted]

开　　本：24 开
印　　张：15
版　　次：2006 年 12
版权登记：图字:01-200

书　　号：7-5062-7304-7/ O · 566　　定　　价：38.00 元

Preface

As was observed previously in the preface to my three-volume work *Group Theory in Physics*, thirty years or so ago group theory could have been regarded by physicists as merely providing a very valuable tool for the elucidation of the symmetry aspects of physical problems. However, recent developments, particularly in high-energy physics, have transformed its role, so that it now occupies a crucial and indispensable position at the centre of the stage. These developments have taken physicists increasingly deeper into the fascinating world of the pure mathematicians, and have led to an ever-growing appreciation of their achievements, the full recognition of which has been hampered to some extent by the style in which much of modern pure mathematics is presented. As with my previous three-volume treatise, one of the main objectives of the present work is to try to overcome this communication barrier, and to present to theoretical physicists and others some of the important mathematical developments in a form that should be easier to comprehend and appreciate.

Although my *Group Theory in Physics* was intended to provide a introduction to the subject, it also aimed to provide a thorough and self-contained account, and so its overall length may well have made it appear rather daunting. The present book has accordingly been designed to provide a much more succinct introduction to the subject, suitable for advanced undergraduate and postgraduate students, and for others approaching the subject for the first time. The treatment starts with the basic concepts and is carried through to some of the most significant developments in atomic physics, electronic energy bands in solids, and the theory of elementary particles. No prior knowledge of group theory is assumed, and, for convenience, various relevant algebraic concepts are summarized in Appendices A and B.

The present work is essentially an abridgement of Volumes I and II of *Group Theory in Physics* (which hereafter will be referred to as "Cornwell (1984)"), although some new material has been included. The intention has been to concentrate on introducing and describing in detail the most important basic ideas and the role that they play in physical problems. Inevitably restrictions on length have meant that some other important concepts and developments have had to be omitted. Nevertheless the mathematical coverage goes outside the strict confines of group theory itself, for one soon is led to the study of Lie algebras, which, although related to Lie groups, are often developed by mathematicians as a separate subject.

Mathematical proofs have been included only when the direct nature of their arguments assist in the appreciation of theorems to which they refer. In other cases references have been given to works in which they may be found. In many instances these references are quoted as "Cornwell (1984)", as interested readers may find it useful to see these proofs with the same notations, conventions, and nomenclature as in the present work. Of course, this is *not* intended to imply that this reference is either the original source or the only place in which a proof may be found. The same reservation naturally applies to the references to suggested further reading on topics that have been explicitly omitted here.

In the text the treatments of specific cases are frequently given under the heading of "Examples". The format is such that these are clearly distinguished from the main part of the text, the intention being that to indicate that the detailed analysis in the Example is not essential for the general understanding of the rest of that section or the succeeding sections. Nevertheless, the Examples are important for two reasons. Firstly, they give concrete realizations of the concepts that have just been introduced. Secondly, they indicate how the concepts apply to certain physically important groups or algebras, thereby allowing a "parallel" treatment of a number of specific cases. For instance, many of the properties of the groups SU(2) and SU(3) are developed in a series of such Examples.

For the benefit of readers who may wish to concentrate on specific applications, the following list gives the relevant chapters:

(i) electronic energy bands in solids: Chapters 1, 2, and 4 to 7;
(ii) atomic physics: Chapters 1 to 6, and 8 to 10;
(iii) elementary particles: Chapters 1 to 6, and 8 to 13.

J.F.Cornwell
St.Andrews
January, 1997

To my wife Elizabeth and my daughters
Rebecca and Jane

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Chapter 1

The Basic Framework

1 The concept of a group

The aim of this chapter is to introduce the idea of a group, to give some physically important examples, and then to indicate immediately how this notion arises naturally in physical problems, and how the related concept of a group representation lies at the heart of the quantum mechanical formulation. With the basic framework established, the next four chapters will explore in more detail the relevant properties of groups and their representations before the application to physical problems is taken up in earnest in Chapter 6.

To mathematicians a group is an object with a very precise meaning. It is a set of elements that must obey four group axioms. On these is based a most elaborate and fascinating theory, not all of which is covered in this book. The development of the theory does not depend on the nature of the elements themselves, but in most physical applications these elements are transformations of one kind or another, which is why T will be used to denote a typical group member.

Definition *Group* $\mathcal{G}$

A set $\mathcal{G}$ of elements is called a "group" if the following four "group axioms" are satisfied:

(a) There exists an operation which associates with every pair of elements T and T' of $\mathcal{G}$ another element T'' of $\mathcal{G}$. This operation is called *multiplication* and is written as $T'' = TT'$, T'' being described as the "product of T with T'".

(b) For any three elements T, T' and T'' of $\mathcal{G}$

$$(TT')T'' = T(T'T''). \tag{1.1}$$

This is known as the "associative law" for group multiplication. (The interpretation of the left-hand side of Equation (1.1) is that the product

TT' is to be evaluated first, and then multiplied by T'' whereas on the right-hand side T is multiplied by the product $T'T''$.)

(c) There exists an *identity element* E which is contained in $\mathcal{G}$ such that

$$TE = ET = T$$

for every element T of $\mathcal{G}$.

(d) For each element T of $\mathcal{G}$ there exists an *inverse element* T^{-1} which is also contained in $\mathcal{G}$ such that

$$TT^{-1} = T^{-1}T = E\,.$$

This definition covers a diverse range of possibilities, as the following examples indicate.

Example I *The multiplicative group of real numbers*
The simplest example (from which the concept of a group was generalized) is the set of all real numbers (excluding zero) with ordinary multiplication as the group multiplication operation. The axioms (a) and (b) are obviously satisfied, the identity is the number 1, and each real number t ($\neq 0$) has its reciprocal $1/t$ as its inverse.

Example II *The additive group of real numbers*
To demonstrate that the group multiplication operation need not have any connection with ordinary multiplication, take $\mathcal{G}$ to be the set of all real numbers with ordinary *addition* as the group multiplication operation. Again axioms (a) and (b) are obviously satisfied, but in this case the identity is 0 (as $a + 0 = 0 + a = a$) and the inverse of a real number a is its negative $-a$ (as $a + (-a) = (-a) + a = 0$).

Example III *A finite matrix group*
Many of the groups appearing in physical problems consist of matrices with matrix multiplication as the group multiplication operation. (A brief account of the terminology and properties of matrices is given in Appendix A.) As an example of such a group let $\mathcal{G}$ be the set of eight matrices

$$\mathbf{M}_1 = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \quad \mathbf{M}_2 = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}, \quad \mathbf{M}_3 = \begin{bmatrix} -1 & 0 \\ 0 & -1 \end{bmatrix},$$

$$\mathbf{M}_4 = \begin{bmatrix} -1 & 0 \\ 0 & 1 \end{bmatrix}, \quad \mathbf{M}_5 = \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix}, \quad \mathbf{M}_6 = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix},$$

$$\mathbf{M}_7 = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad \mathbf{M}_8 = \begin{bmatrix} 0 & -1 \\ -1 & 0 \end{bmatrix}.$$

By explicit calculation it can be verified that the product of any two members of $\mathcal{G}$ is also contained in $\mathcal{G}$, so that axiom (a) is satisfied. Axiom (b) is automatically true for matrix multiplication, M_1 is the identity of axiom (c) as it is a unit matrix, and finally axiom (d) is satisfied as

$$\begin{array}{llll} \mathbf{M}_1^{-1} = \mathbf{M}_1, & \mathbf{M}_2^{-1} = \mathbf{M}_2, & \mathbf{M}_3^{-1} = \mathbf{M}_3, & \mathbf{M}_4^{-1} = \mathbf{M}_4, \\ \mathbf{M}_5^{-1} = \mathbf{M}_6, & \mathbf{M}_6^{-1} = \mathbf{M}_5, & \mathbf{M}_7^{-1} = \mathbf{M}_7, & \mathbf{M}_8^{-1} = \mathbf{M}_8. \end{array}$$

Example IV *The groups* U(N) *and* SU(N)
U(N) for $N \geq 1$ is defined to be the set of all $N \times N$ unitary matrices $\mathbf{u}$ with matrix multiplication as the group multiplication operation. SU(N) for $N \geq 2$ is defined to be the subset of such matrices $\mathbf{u}$ for which $\det \mathbf{u} = 1$, with the same group multiplication operation. (As noted in Appendix A, if $\mathbf{u}$ is unitary then $\det \mathbf{u} = \exp(i\alpha)$, where α is some real number. The "S" of SU(N) indicates that SU(N) is the "special" subset of U(N) for which this α is zero.)

It is easily established that these sets do form groups. Consider first the set U(N). As $(\mathbf{u}_1\mathbf{u}_2)^\dagger = \mathbf{u}_2^\dagger\mathbf{u}_1^\dagger$ and $(\mathbf{u}_1\mathbf{u}_2)^{-1} = \mathbf{u}_2^{-1}\mathbf{u}_1^{-1}$, if $\mathbf{u}_1$ and $\mathbf{u}_2$ are both unitary then so is $\mathbf{u}_1\mathbf{u}_2$. Again axiom (b) is automatically valid for matrix multiplication and, as the unit matrix $\mathbf{1}_N$ is a member of U(N), it provides the identity E of axiom (c). Finally, axiom (d) is satisfied, as if $\mathbf{u}$ is a member of U(N) then so is $\mathbf{u}^{-1}$.

For SU(N) the same considerations apply, but in addition if $\mathbf{u}_1$ and $\mathbf{u}_2$ both have determinant 1, Equation (A.4) shows that the same is true of $\mathbf{u}_1\mathbf{u}_2$. Moreover, $\mathbf{1}_N$ is a member of SU(N), so it is its identity, and $\mathbf{u}^{-1}$ is a member of SU(N) if that is the case for $\mathbf{u}$.

The set of groups SU(N) is particularly important in theoretical physics. SU(2) is intimately related to angular momentum and isotopic spin, as will be shown in Chapters 10 and 13, while SU(3) is now famous for its role in the classification of elementary particles, which will also be studied in Chapter 13.

Example V *The groups* O(N) *and* SO(N)
The set of all $N \times N$ real orthogonal matrices $\mathbf{R}$ (for $N \geq 2$) is denoted almost universally by O(N), although O($N, \mathbb{R}$) would have been preferable as it indicates that only real matrices are included. The subset of such matrices $\mathbf{R}$ with $\det \mathbf{R} = 1$ is denoted by SO(N). As will be described in Section 2, O(3) and SO(3) are intimately related to rotations in a real three-dimensional Euclidean space, and so occur time and time again in physical applications.

O(N) and SO(N) are both groups with matrix multiplication as the group multiplication operation, as they can be regarded as being the subsets of U(N) and SU(N) respectively that consist only of real matrices. (All that has to be observed to supplement the arguments given in Example IV is that the product of any two real matrices is real, that $\mathbf{1}_N$ is real, and that the inverse of a real matrix is also real.)

If $T_1T_2 = T_2T_1$ for *every* pair of elements T_1 and T_2 of a group $\mathcal{G}$ (that is, if all T_1 and T_2 of $\mathcal{G}$ *commute*), then $\mathcal{G}$ is said to be "Abelian". It will transpire

	$\mathbf{M}_1$	$\mathbf{M}_2$	$\mathbf{M}_3$	$\mathbf{M}_4$	$\mathbf{M}_5$	$\mathbf{M}_6$	$\mathbf{M}_7$	$\mathbf{M}_8$
$\mathbf{M}_1$	$\mathbf{M}_1$	$\mathbf{M}_2$	$\mathbf{M}_3$	$\mathbf{M}_4$	$\mathbf{M}_5$	$\mathbf{M}_6$	$\mathbf{M}_7$	$\mathbf{M}_8$
$\mathbf{M}_2$	$\mathbf{M}_2$	$\mathbf{M}_1$	$\mathbf{M}_4$	$\mathbf{M}_3$	$\mathbf{M}_8$	$\mathbf{M}_7$	$\mathbf{M}_6$	$\mathbf{M}_5$
$\mathbf{M}_3$	$\mathbf{M}_3$	$\mathbf{M}_4$	$\mathbf{M}_1$	$\mathbf{M}_2$	$\mathbf{M}_6$	$\mathbf{M}_5$	$\mathbf{M}_8$	$\mathbf{M}_7$
$\mathbf{M}_4$	$\mathbf{M}_4$	$\mathbf{M}_3$	$\mathbf{M}_2$	$\mathbf{M}_1$	$\mathbf{M}_7$	$\mathbf{M}_8$	$\mathbf{M}_5$	$\mathbf{M}_6$
$\mathbf{M}_5$	$\mathbf{M}_5$	$\mathbf{M}_7$	$\mathbf{M}_6$	$\mathbf{M}_8$	$\mathbf{M}_3$	$\mathbf{M}_1$	$\mathbf{M}_4$	$\mathbf{M}_2$
$\mathbf{M}_6$	$\mathbf{M}_6$	$\mathbf{M}_8$	$\mathbf{M}_5$	$\mathbf{M}_7$	$\mathbf{M}_1$	$\mathbf{M}_3$	$\mathbf{M}_2$	$\mathbf{M}_4$
$\mathbf{M}_7$	$\mathbf{M}_7$	$\mathbf{M}_5$	$\mathbf{M}_8$	$\mathbf{M}_6$	$\mathbf{M}_2$	$\mathbf{M}_4$	$\mathbf{M}_1$	$\mathbf{M}_3$
$\mathbf{M}_8$	$\mathbf{M}_8$	$\mathbf{M}_6$	$\mathbf{M}_7$	$\mathbf{M}_5$	$\mathbf{M}_4$	$\mathbf{M}_2$	$\mathbf{M}_3$	$\mathbf{M}_1$

Table 1.1: Multiplication table for the group of Example III.

that such groups have relatively straightforward properties. However, many of the groups having physical applications are non-Abelian. Of the cases considered above the only Abelian groups are those of Examples I and II and the groups U(1) and SO(2) of Examples IV and V. (One of the non-commuting pairs of products of Example III which makes that group non-Abelian is $\mathbf{M}_5\mathbf{M}_7 = \mathbf{M}_4$, $\mathbf{M}_7\mathbf{M}_5 = \mathbf{M}_2$.)

The "order" of $\mathcal{G}$ is defined to be the number of elements in $\mathcal{G}$, which may be finite, countably infinite, or even non-countably infinite. A group with finite order is called a "finite group". The vast majority of groups that arise in physical situations are either finite groups or are "Lie groups", which are a special type of group of non-countably infinite order whose precise definition will be given in Chapter 3, Section 1. Example III is a finite group of order 8, whereas Examples I, II, IV and V are all Lie groups.

For a finite group the product of every element with every other element is conveniently displayed in a multiplication table, from which all information on the structure of the group can subsequently be deduced. The multiplication table of Example III is given in Table 1.1. (By convention the order of elements in a product is such that the element in the left-hand column precedes the element in the top row, so for example $\mathbf{M}_5\mathbf{M}_8 = \mathbf{M}_2$.) For groups of infinite order the construction of a multiplication table is clearly completely impractical, but fortunately for a Lie group the structure of the group is very largely determined by another finite set of relations, namely the commutation relations between the basis elements of the corresponding real Lie algebra, as will be explained in detail in Chapter 8.

2 Groups of coordinate transformations

To proceed beyond an intuitive picture of the effect of symmetry operations, it is necessary to specify the operations in a precise algebraic form so that the results of successive operations can be easily deduced. Attention will be confined here to transformations in a real three-dimensional Euclidean space $\mathbb{R}^3$, as most applications in atomic, molecular and solid state physics involve only transformations of this type.

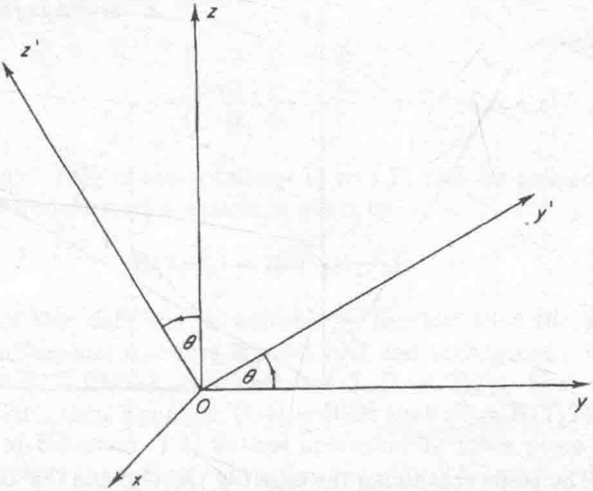

Figure 1.1: Effect of a rotation through an angle θ in the right-hand screw sense about Ox.

(a) Rotations

Let Ox, Oy, Oz be three mutually orthogonal Cartesian axes and let Ox', Oy', Oz' be another set of mutually orthogonal Cartesian axes with the same origin O that is obtained from the first set by a rotation T about a specified axis through O. Let (x, y, z) and (x', y', z') be the coordinates of a fixed point P in the space with respect to these two sets of axes. Then there exists a real orthogonal 3×3 matrix $\mathbf{R}(T)$ which depends on the rotation T, but which is independent of the position of P, such that

$$\mathbf{r}' = \mathbf{R}(T)\mathbf{r}, \tag{1.2}$$

where

$$\mathbf{r}' = \begin{bmatrix} x' \\ y' \\ z' \end{bmatrix} \text{ and } \mathbf{r} = \begin{bmatrix} x \\ y \\ z \end{bmatrix}.$$

(Hereafter position vectors will always be considered as 3×1 column matrices in matrix expressions unless otherwise indicated, although for typographical reasons they will often be displayed in the text as 1×3 row matrices.) For example, if T is a rotation through an angle θ in the right-hand screw sense about the axis Ox, then, as indicated in Figures 1.1 and 1.2,

$$\begin{aligned} x' &= x, \\ y' &= y\cos\theta + z\sin\theta, \\ z' &= -y\sin\theta + z\cos\theta, \end{aligned}$$

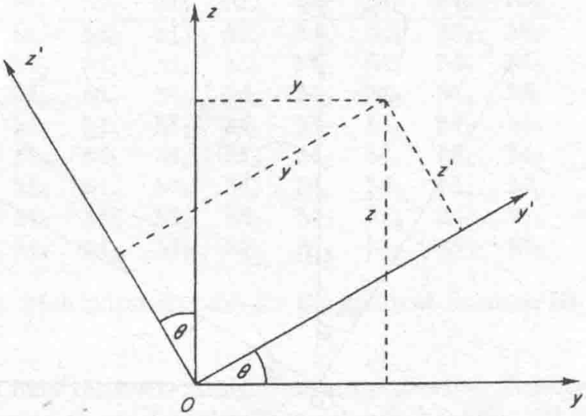

Figure 1.2: The plane containing the axes Oy, Oz, Oy' and Oz' corresponding to the rotation of Figure 1.1.

so that

$$\mathbf{R}(T) = \begin{bmatrix} 1 & 0 & 0 \\ 0 & \cos\theta & \sin\theta \\ 0 & -\sin\theta & \cos\theta \end{bmatrix}. \tag{1.3}$$

The matrix $\mathbf{R}(T)$ obeys the orthogonality condition $\widetilde{\mathbf{R}}(T) = \mathbf{R}(T)^{-1}$ because rotations leave invariant the length of every position vector and the angle between every pair of position vectors, that is, they leave invariant the scalar product $\mathbf{r}_1.\mathbf{r}_2$ of any two position vectors. (Indeed the name "orthogonal" stems from the involvement of such matrices in the transformations being considered here between sets of orthogonal axes.) The proof that $\mathbf{R}(T)$ is orthogonal depends on the fact that $\mathbf{r}_1.\mathbf{r}_2$ can be expressed in matrix form as $\widetilde{\mathbf{r}}_1\mathbf{r}_2$. Then, if $\mathbf{r}'_1 = \mathbf{R}(T)\mathbf{r}_1$ and $\mathbf{r}'_2 = \mathbf{R}(T)\mathbf{r}_2$, it follows that $\mathbf{r}'_1.\mathbf{r}_2 = \widetilde{\mathbf{r}}'_1\mathbf{r}'_2 = \widetilde{\mathbf{r}}_1\widetilde{\mathbf{R}}(T)\mathbf{R}(T)\mathbf{r}_2$, which is equal to $\widetilde{\mathbf{r}}_1\mathbf{r}_2$ for all $\mathbf{r}_1$ and $\mathbf{r}_2$ if and only if $\widetilde{\mathbf{R}}(T)\mathbf{R}(T) = \mathbf{1}$.

As noted in Appendix A, the orthogonality condition implies that $\det \mathbf{R}(T)$ can take only the values $+1$ or -1. If $\det \mathbf{R}(T) = +1$ the rotation is said to be "proper"; otherwise it is said to be "improper". The only rotations which can be applied to a rigid body are proper rotations. The transformation of Equation (1.3) gives an example.

The simplest example of an improper rotation is the spatial inversion operation I for which $\mathbf{r}' = -\mathbf{r}$, so that

$$\mathbf{R}(I) = \begin{bmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{bmatrix}.$$

Another important example is the operation of reflection in a plane. For instance, for reflection in the plane Oyz, for which $x' = -x, y' = y, z' = z$,