ANGULAR MOMENTUM

An Illustrated Guide to Rotational Symmetries for Physical Systems

WILLIAM J. THOMPSON

University of North Carolina Chapel Hill, North Carolina



WILEY-VCH Verlag GmbH & Co. KGaA

This Page Intentionally Left Blank

ANGULAR MOMENTUM

This Page Intentionally Left Blank

ANGULAR MOMENTUM

An Illustrated Guide to Rotational Symmetries for Physical Systems

WILLIAM J. THOMPSON

University of North Carolina Chapel Hill, North Carolina



WILEY-VCH Verlag GmbH & Co. KGaA

All books published by Wiley-VCH are carefully produced. Nevertheless, authors, editors, and publisher do not warrant the information contained in these books, including this book, to be free of errors. Readers are advised to keep in mind that statements, data, illustrations, procedural details or other items may inadvertently be inaccurate.

Library of Congress Card No.:

Applied for

British Library Cataloging-in-Publication Data:

A catalogue record for this book is available from the British Library

Bibliographic information published by Die Deutsche Bibliothek

Die Deutsche Bibliothek lists this publication in the Deutsche Nationalbibliografie; detailed bibliographic data is available in the Internet at http://dnb.ddb.de>.

© 1994 by John Wiley & Sons, Inc. © 2004 WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim

All rights reserved (including those of translation into other languages). No part of this book may be reproduced in any form – nor transmitted or translated into machine language without written permission from the publishers. Registered names, trademarks, etc. used in this book, even when not specifically marked as such, are not to be considered unprotected by law.

Printed in the Federal Republic of Germany Printed on acid-free paper

Printing Strauss GmbH, Mörlenbach **Bookbinding** Litges & Dopf Buchbinderei GmbH, Heppenheim

ISBN-13: 978-0-471-55264-2 **ISBN-10:** 0-471-55264-X



CONTENTS

Pı	xi				
The Computer Interface					
1	Sym	metry in Physical Systems	1		
	1.1	Symmetries and invariances 1 1.1.1 Symmetries and conservation laws 2 1.1.2 Noether's theorem and Curie's principle 5			
	1.2	Spatial symmetries 7 1.2.1 Reflection symmetry in nature 8 1.2.2 Translation symmetries; mosaics and crystals 10			
	1.3	Rotational symmetries 12 1.3.1 Active and passive rotations; Euler angles 13 1.3.2 Coordinate systems for rotations 17 1.3.3 Angular momentum and rotations: a cameo portrait 19			
	1.4	Discrete symmetries and quantum systems 21 1.4.1 Parity symmetry 22 1.4.2 Charge conjugation and time reversal 25 1.4.3 Maxwell's equations and <i>PCT</i> 30 1.4.4 <i>PCT</i> and the Pauli principle: Lüder's theorem 32			
	1.5	Broken symmetries from cosmetology to cosmology 34 Problems on symmetry in physical systems 36			

v i CONTENTS

2 Mathematical and Quantal Preliminaries

- 2.1 Matrix definitions and manipulations 42
 - 2.1.1 Linear spaces and operator matrix elements 42
 - 2.1.2 Inner and direct products of matrices 45
 - 2.1.3 Operations on matrices, and special properties 50
 - 2.1.4 Phase manipulation rules 52
- 2.2 Transformations and operators 53
 - 2.2.1 Similarity and symmetry transformations 53
 - 2.2.2 Unitarity: its interpretation in quantum mechanics 57
 - 2.2.3 Operator exponentials and commutators 58
 - 2.2.4 Raising and lowering operators 59
- 2.3 Eigenvalues and eigenstates 63
 - 2.3.1 Eigenvalues of operators and matrices 63
 - 2.3.2 Diagonalizing matrices 64
 - 2.3.3 Eigenvectors as basis states 66
- 2.4 Spinors and their properties 67
 - 2.4.1 Definitions of spinors 67
 - 2.4.2 Representing spinors; rotations 69
 - 2.4.3 Objects that distinguish turns though 2π and 4π 72
- 2.5 A primer on groups 72
 - 2.5.1 Group examples and definitions 73
 - 2.5.2 Group theory terminology 79
 - 2.5.3 Representations of groups 80
 - 2.5.4 Interesting groups and their uses 84
 - 2.5.5 Irreducibility of a representation 88
- 2.6 Mathematics, groups, and the physical sciences 89

Problems on mathematical and quantal preliminaries 90

3 Rotational Invariance and Angular Momentum

- 3.1 Infinitesimal rotations; the J operators 95
 - 3.1.1 Schemes for describing rotations 96
 - 3.1.2 Commutation relations of J operators 97
 - 3.1.3 The spherical-basis operators J_{+1} , J_0 , J_{-1} 99
- 3.2 Orbital angular momentum operators 100
 - 3.2.1 Infinitesimal rotations applied to spatial functions 100
 - 3.2.2 Components of L in spherical polar coordinates 103
 - 3.2.3 The special role of the operator L_z 105
- 3.3 Other representations of **J** operators 105
 - 3.3.1 The 2×2 matrix representation: Pauli matrices 105
 - 3.3.2 Eigenvectors of the Pauli matrices 108
 - 3.3.3 Finite rotations and Pauli matrices 109
 - 3.3.4 Spinor space and its operators 111
- 3.4 Angular momentum eigenvalues and matrix elements 113
 - 3.4.1 Eigenvalues of J^2 and J_z ; irreducibility 113
 - 3.4.2 Matrix elements in the spherical basis 116
 - 3.4.3 Matrix elements in the Cartesian basis 117
 - 3.4.4 Operator matrices for j = 1/2, 1, and 3/2 119
 - 3.4.5 Angular momentum: geometrical and dynamical 120

95

127

169

211

3.5 Reference frames: spin and orbital angular momenta 122 Problems on rotational invariance and angular momentum 124

4 Angular Momentum Eigenstates

- 4.1 Orbital eigenstates and spherical harmonics 127
 - 4.1.1 Legendre functions and their properties 129
 - 4.1.2 Displaying Legendre functions; polar diagrams 131
 - 4.1.3 Calculating and visualizing spherical harmonics 135
 - 4.1.4 Solid harmonics and other variants 143
- 4.2 Spherical-basis vectors and angular momentum in a field 149
 - 4.2.1 Vectors in the spherical basis 150
 - 4.2.2 Infinitesimal rotations of vectors 152
 - 4.2.3 The electromagnetic field and photons 155
- 4.3 Spin eigenstates and their representations 156
 - 4.3.1 What is spin? 156
 - 4.3.2 Intrinsic spin eigenstates 160
 - 4.3.3 Spinor-space representations 162
 - 4.3.4 Time reversal and spin 163
 - Problems on angular momentum eigenstates 165

5 Angular Momentum in Quantum Systems

5.1 Rotational symmetry and dynamical angular momentum 170

- 5.1.1 Angular momentum and the role of Planck's constant 170
- 5.1.2 Classical angular momentum: Ehrenfest theorems 172
- 5.1.3 Larmor precession in magnetic fields 175
- 5.2 Uncertainty relations for angular momentum 179
 - 5.2.1 Heisenberg uncertainty relations for quantum systems 180
 - 5.2.2 Angular momentum uncertainties 183
 - 5.2.3 Uncertainties between angular momentum and angles 186
- 5.3 The semiclassical vector model 189
 - 5.3.1 Constructing the vector model of angular momentum 190
 - 5.3.2 Uses and limitations of the vector model 192
- 5.4 Angular momentum and wave mechanics 193
 5.4.1 Plane waves and centripetal barriers; Bessel functions 193
 5.4.2 Displaying partial-wave expansions 199
- 5.5 The conceptual development of angular momentum 203 Problems on angular momentum in quantum systems 206

6 Finite Rotations of Angular Momentum Eigenstates

- 6.1 Introduction to rotation matrices 211
 - 6.1.1 Review of rotations and angle schemes 212
 - 6.1.2 Group and factorization properties of rotations 213

- 6.2 Determining rotation matrices 213
 - 6.2.1 Rotation of eigenstates about z axes 214
 - 6.2.2 Rotations about the y axis for j = 1 216
 - 6.2.3 Constructing d from spinor representations 218
 - 6.2.4 Relation of d^{j} elements to other functions 220
 - 6.2.5 Computing reduced rotation matrix elements 222
- 6.3 Interpreting rotated states 224
 - 6.3.1 Orbital angular momentum states 225
 - 6.3.2 Transformation amplitudes for arbitrary j 227
 - 6.3.3 Visualizing rotation matrix elements 230
- 6.4 Properties of rotation matrices 232
 - 6.4.1 Symmetry properties of d^{j} and D^{j} 232
 - 6.4.2 Unitarity and orthogonality properties 234
 - 6.4.3 Classical limits of rotation matrices 236
 - 6.4.4 Spherical harmonics as rotation matrix elements 239.
- 6.5 Rigid-body rotations in quantum mechanics 240
 - 6.5.1 The D^{j} as angular momentum eigenfunctions 241
 - 6.5.2 The Hamiltonian of a rigid rotator 242
 - 6.5.3 Rotational states of molecules and nuclei 245
 - Problems on finite rotations of angular momentum eigenstates 247

7 Combining Two Angular Momentum Eigenstates

251

- 7.1 The semiclassical vector model for addition 252
 - 7.1.1 Vector-addition construction 252
 - 7.1.2 Triangle and projection selection rules 253
 - 7.1.3 Interpreting coupling: spin-orbit interaction 255
 - 7.1.4 Degeneracy of energy states in the Coulomb potential 258
- 7.2 Coupling coefficients: definitions and general properties 263
 - 7.2.1 Combining two angular momenta: Clebsch-Gordan coefficients 264
 - 7.2.2 Unitarity of Clebsch-Gordan coefficients 264
 - 7.2.3 Determining coefficients from spinor representations 266
- 7.3 The 3-*j* coefficients and their properties 269
 - 7.3.1 Three angular momenta coupled to zero; 3-j coefficients 269
 - 7.3.2 Visualizing symmetry properties 276
 - 7.3.3 Classical limits of 3-j coefficients 278
 - 7.3.4 Expressions for one angular momentum small 280
- 7.4 Computing coupling coefficients 280
 - 7.4.1 Tabulations of coupling coefficients 281
 - 7.4.2 Computing 3-j coefficients efficiently 282
- 7.5 Rotation matrices and coupling coefficients 286
 - 7.5.1 Clebsch-Gordan series for combining D^{j} elements 286
 - 7.5.2 Special cases of Clebsch-Gordan series 288
 - 7.5.3 Integrals of rotation functions 292
 - 7.5.4 Examples: Celestial bodies and rotator matrix elements 295

Problems on combining two angular momentum eigenstates 300

8	Irre	ducible Spherical Tensors and Spin	305	
	8.1 Definition of irreducible tensor operators 308			
		8.1.1 Defining irreducible spherical tensors 308 8.1.2 Bacab's definition and its applications 309		
	82	Combining irreducible tensors 312		
	0.2	8.2.1 Building up irreducible spherical tensors 312		
		8.2.2 Contraction of irreducible tensors to scalars 315		
	8.3	Wigner-Eckart theorem; reduced matrix elements 316		
		8.3.1 Geometry and dynamics: The Wigner-Eckart theorem 317		
		8.3.2 Conventions for reduced matrix elements 320		
	0.4	8.3.3 Determining and using reduced matrix elements 320		
	8.4	8.4 Density matrices and polarization tensors 325		
		8.4.1 Spin density matrices and spin tensors 325 8.4.2 Spin precession in magnetic fields: rotating frames 330		
		8.4.3 Spin procession in magnetic field gradients 335		
		Problems on irreducible spherical tensors and spin 341		
a	Rec	ombining Several Angular Momentum Figuretates	315	
1	0 1	Decoupling three angular momenta 345	343	
	9.1	9.1.1. Receipting times angular momenta 345		
		9.1.2 Recoupling tetrahedra, quadrilaterals, and trees 348		
	9.2	Formulas for 6-j coefficients 350		
		9.2.1 Expansion in terms of 3-j coefficients 350		
		9.2.2 Algebraic expressions for 6- <i>j</i> coefficients 352		
	0.2	9.2.3 Tabulations of 6-j coefficients 354		
	9.3	Properties of recoupling coefficients 354		
		9.3.2 Symmetries and special values of 6- <i>i</i> coefficients 355		
		9.3.3 Computing 6- <i>j</i> coefficients efficiently 359		
	9.4	Scalar products of irreducible tensors 361		
		9.4.1 Factorization and projection theorems for tensors 361		
		9.4.2 Matrix elements of multipole expansions 365		
	o -	9.4.3 Tensors in $L-S$ and $j-j$ coupling schemes 367		
	9.5	Recoupling four angular momenta 370		
		9.5.1 Definition and computation of 9-j coefficients 370		
		9.5.3 Tensor matrix elements in coupled schemes 376		
		9.5.4 Transformations between $L - S$ and $j - j$ coupling 377		
		9.5.5 Graphical and automated methods 380		
		Problems on recombining several angular momentum eigenstates 38	31	

EPILOGUE

385

APPENDIX I NOTEBOOKS FOR MATHEMATICA 387

APPENDIX II NUMERICAL COMPUTER PROGRAMS IN C 407 C1 Program for reduced rotation matrix elements 410 C2 Program for 3-*j* coefficients 412 C3 Program for 6-*j* coefficients 415 C4 Program for 9-*j* coefficients 417 APPENDIX III TABLES OF FORMULAS 421 **T**1 Legendre functions and spherical harmonics 421 T2 Rotation matrix elements 423 T3 The 3-*j* coefficients 425 Irreducible spherical tensor operators 429 T4 T5 The 6-*j* coefficients 431 T6 The 9-*i* coefficients 433 REFERENCES 437

INDEX

449



PREFACE

If a physical system has only internal interactions and if space is isotropic, then intrinsic properties of the system must be independent of its orientation and must be indistinguishable in all directions. From this fundamental rotational symmetry concept the theory of angular momentum has been developed into a sophisticated analytical and computational technique, especially when applied to quantum mechanics. I aim in this book to develop angular momentum theory in a pedagogically consistent way, starting from the geometrical concept of rotational invariance rather than from the dynamical idea of orbital angular momentum and its quantization. The latter approach, though hallowed by tradition, needlessly confuses quantum mechanics with geometry.

Topics are presented in an order so that new concepts are introduced and relevant formulas are derived in ways arising naturally in the treatment rather than by appealing to unfamiliar concepts or *ad hoc* methods. Modern notation and terminology are used in a geometric and algebraic approach. Some concepts of group theory are introduced and are related to this approach, but knowledge of group theory is not required. Those who plan to use continuous groups that are more abstract than the rotation group may thereby develop their insight and skills by practicing with rotations. I try to distinguish carefully results that depend only on rotational symmetry and are generally valid from those having their most fruitful interpretation from the viewpoint of quantum mechanics. Applications to quantum mechanics therefore usually appear toward the end of sections and chapters.

Although Angular Momentum is intended to be pedagogically self-contained, the treatment is not encyclopedic, since broad-ranging surveys of angular momentum theory and extensive tabulations of formulas are now available. There is also a large research literature for further study, to which I direct you. Indeed, the field of angular momentum theory has become a mecca for algebraists. In this book, I prefer to emphasize concepts rather than techniques, because imagination is usually more important than knowledge, even in the sciences.

Visualization of objects and quantities being rotated is important for insightful and practical use of the concepts and methods of rotational symmetry. I therefore provide nearly 130 illustrations to help you understand what the mathematics is describing. If you have access to a computer software system combining mathematics and graphics, such as *Mathematica* or *Maple*, you too may explore such visualizations. There are 26 program notebooks—used to generate indicated figures in the text and for parts of the problem section at the end of each chapter—provided in Appendix I. Although written for *Mathematica* on an Apple Macintosh computer, they are readily adaptable to *Maple*.

Practical aspects are not neglected. For example, we discuss how to compute coupling coefficients efficiently, while computer programs for numerical evaluation of reduced rotation matrix elements and for 3-*j*, 6-*j*, and 9-*j* coefficients are given in Appendix II. These programs are written in the C language and are designed to be readily adaptable to Fortran and Pascal. Tables of formulas for practical reference are collected in Appendix III.

For use as a textbook, *Angular Momentum* assumes knowledge of mathematics through matrix algebra and differential equations, plus understanding of quantum mechanics usually acquired in one year of course work. Thus, I hope to make the subject of rotational symmetry accessible to advanced undergraduates in chemistry, physics, and mathematics. From several years experience of teaching courses using the materials in *Angular Momentum*, I have found that the book can readily be comprehended in less than a half year of course work, even when supplemented by detailed examples from the specific discipline in which it is taught. Emphasis is placed throughout on appropriate interpretation and use of derived results. To help with self-study and to test comprehension, 135 problems at the end of the chapters can be used to reinforce concepts and to improve skills.

Angular Momentum should provide suitable preparation for applications to research in the physical sciences—especially in physics, chemistry, and related areas of mathematical physics, such as group theory. Extensive references are given to material that is more advanced in concepts and techniques, as well as to applications of rotational symmetry aspects in research on physical systems.

Although a book may be the offspring of a single author, it has many midwives. A generation of students has helped me to refine my ideas on the subject, the U.S. Department of Energy unwittingly provided some financial support, while Ms. Word and Mac Intosh patiently retyped many drafts of the text and helped prepare the illustrations. Professors Louise Dolan and Charles Poole reviewed the manuscript and gave many suggestions for improvements. Greg Franklin and Bob Hilbert at Wiley-Interscience helped expedite the publication.

WILLIAM J. THOMPSON

Chapel Hill, February 1994



THE COMPUTER INTERFACE

The interface between angular momentum theory and computers occurs at two levels; conceptual and technical. At the conceptual level, computers are useful to visualize functions describing rotational symmetries and to produce algebraic formulas correctly and rapidly. At the technical level, we need algebraic and numerical results for functions describing these symmetries, and these results are obtained most efficiently by using computers.

Conceptual aspects of angular momentum that are helped by the interface to computers include illustration of angular momentum eigenstates (Section 4.1), of partial-wave expansions (Section 5.4), of rotation matrix elements and their classical limits (Sections 6.3 and 6.4), and of spin precession in magnetic fields (Section 8.4). Such visualizations are best produced interactively so that you can vary viewpoints and parameters in real time. These visualizations usually require computing algebraic (symbolic) expressions before numerical and graphical results are obtained.

The Mathematica Interface. The computer system we use for conceptual aspects of our treatment is Mathematica, a general-purpose system for doing mathematics by computer. It has convenient visualization capabilities and is available on many computers. In Appendix I we provide Mathematica programs in "notebook" form that are immediately usable on several small computers and on workstations. Mathematica is described in several books, such as Maeder's [Mae91] and Wolfram's [Wol91]. The programs are written to make them easy to translate to other programming environments, such as the Maple system for symbolic, numerical, and graphical computation. Introductions to Maple are provided in the book by

Char et al. [Cha92] and in Heck's book [Hec92]. Both *Maple* and *Mathematica* provide facilities for translating their symbolic output into C or Fortran code.

Technical aspects of rotational symmetries for physical systems typically require algebraic or numerical evaluation of functions describing eigenstates (Chapter 4), partial-wave expansions (Section 5.4), rotation matrices (Chapter 6), and coupling coefficients (Chapters 7 and 9). For exploratory use, the 26 *Mathematica* programs in Appendix I are suitable.

Problems at the end of each chapter that suggest using one of the *Mathematica* notebooks are indicated by a superscript M, such as 1.2^{M} .

The C Interface. For numerical computations, Appendix II has four programs of moderate efficiency for reduced rotation matrix elements and for 3-j, 6-j, and 9-j coefficients. These are coded in the C programming language, which is available on many computers. The C functions are intended to be incorporated into programs, so we provide just a small driver program that enables the functions to be checked for numerical correctness. If high efficiency is needed for computing coupling coefficients, then the discussions in Sections 7.4.2 (for 3-j coefficients), 9.3.3 (for 6-j coefficients), and 9.5.1 (for 9-j coefficients) will guide you to the technical literature.

The Program Diskette. All the Mathematica and C programs in Appendices I and II are provided on the diskette accompanying this book. The 3.5-inch doubledensity diskette can be read by Apple Macintosh computers, as well as by several other computers with appropriate hardware and software. A general-purpose way of translating from this diskette to diskettes for other computers is suggested in the following diagram.



First, read the Macintosh diskette provided, by using any Macintosh computer that is connected by modem to the other computer, then use the Macintosh to translate all the files on the diskette to ASCII text files. Next, transfer the files over a network to the other computer. Then, in this computer do any editing of the files that is needed to produce the correct format for *Mathematica* or C on that machine. Finally, make copies of the diskette for this computer system.

Chapter 1



SYMMETRY IN PHYSICAL SYSTEMS

The major topic of this book is the study of rotational symmetry applied to physical systems. The five sections in this chapter emphasize the relation between symmetries and invariances in dynamical systems (Section 1.1), the nature of spatial symmetries (Section 1.2), and particularly rotational symmetries (Section 1.3). In Section 1.4 we review the discrete symmetry operations—parity (P), charge conjugation (C), and time reversal (T)—all important in quantum mechanics. Here we also introduce the main ideas of the Pauli and Lüder *PCT* theorem, illustrating it with Maxwell's equations. The Pauli exclusion principle is also involved in these discussions, so we review what is known about the limits of its validity. Finally in this chapter, Section 1.5 is an excursion to look at symmetry and broken symmetries from cosmetology to cosmology.

After completing this chapter, especially if you work the problems at the end, you should have a good idea of the importance of symmetry properties for studying physical systems. In subsequent chapters we expand the concepts of this chapter, using the mathematics summarized in Chapter 2. We try throughout to distinguish considerations which are general and primarily geometrical from those which have their most fruitful applications in quantum mechanics and are primarily dynamical.

1.1 SYMMETRIES AND INVARIANCES

We begin by illustrating the relation of symmetry properties to invariances (conservation laws) of dynamical systems—using in Section 1.1.1 examples from nonrelativistic classical mechanics: linear momentum, total energy, and angular momentum. In Section 1.1.2 we discuss the generalization of these continuous symmetries to Noether's theorem, and we also discuss Curie's symmetry principle.

2 SYMMETRY IN PHYSICAL SYSTEMS

1.1.1 Symmetries and Conservation Laws

We present here examples of the relation between symmetries and conservation laws in the context of classical mechanics. In the following subsection these are generalized to Noether's theorem, which holds for a very wide range of continuous symmetries. What are the relations between symmetry properties of a physical system and conservation laws? To answer this, we consider the time dependence of integrals of the motion [Gol80] for several simple examples from nonrelativistic mechanics.

You should understand that the following examples are interesting because of relationships they illustrate between symmetries and conservation laws rather than because of any manipulative techniques their derivations require or because of the formal results. Indeed, you know the formulas already; it's the spin we put on them that matters. Therefore, most of the details are suggested as problems.

Momentum Conservation. Consider first the one-dimensional case of a single particle having momentum P in the x direction and moving in an *external* potential V(x). Suppose that when we move the particle the potential is unchanged. The time rate of change of its momentum, \dot{P} , is then given by

$$\dot{P} = -\frac{dV}{dx} = 0 \implies P \text{ conserved}$$
 (1.1)

This is fairly obvious, being an example of Newton's law of inertia.

Now consider—again in one dimension for simplicity—two particles interacting only through a *mutual* potential, $V(x_1-x_2)$, that depends only on their separation $x_{12} = x_1-x_2$, independent of the choice of origin, as shown in Figure 1.1. The total



FIGURE 1.1 If two particles interact through a mutual potential depending only on their separation x_{12} , independent of the choice of origin O, then the total momentum is conserved.

momentum of the two-particle system changes with time according to

$$\dot{P} = -\frac{dV}{dx_{12}} - \frac{dV}{dx_{21}} = 0 \implies P \text{ conserved}$$
 (1.2)

This is just an example of Newton's law of action and reaction. If this system is moved as a unit through a displacement X so that

$$x'_1 = x_1 + X$$
 $x'_2 = x_2 + X$ $x'_{12} = x_{12}$ (1.3)

then (1.2) will still hold and symmetry under spatial translation will also result in

conservation of momentum. The general case—three dimensions and a manyparticle system interacting through two-body potentials satisfying the action-reaction condition—requires only technical competence with vector calculus, so we relegate it to Problem 1.1.

Total Energy Conservation. We again start with a simple example—motion of a single particle in one dimension. To consider the time evolution of the system we must assume that the particle is moving in a *time-independent* external potential, V, but now V may depend upon position x. For example, as hinted in Figure 1.2, the external potential may be gravity.



FIGURE 1.2 If a particle moves in an external time-independent potential that may depend on position x, such as gravity, its total energy is conserved.

The total energy of the particle, *E*, may be expressed as

$$E = \frac{1}{2}m\dot{x}^2 + V$$
 (1.4)

Its energy therefore depends on time as

$$\dot{E} = m\dot{x}\frac{d\dot{x}}{dt} + \frac{dV}{dx}\dot{x}$$
(1.5)

By using Newton's force law, we can convert the first term into the negative of the second term, producing

$$\dot{E} = 0 \implies E \text{ conserved}$$
(1.6)

Thus, invariance of the potential energy under continuous time displacements pro-

4 SYMMETRY IN PHYSICAL SYSTEMS

duces conservation of total energy. To prove the general case in three dimensions with a many-particle system interacting through time-independent potentials is suggested in Problem 1.1.

Angular Momentum Conservation. We now turn to the topic of this book, considering the simplest case of mechanical angular momentum—a particle moving in an x - y plane under a *central* potential with no explicit time dependence. This situation has V(x, y, t) = V(r), where $r = \sqrt{(x^2 + y^2)}$. An example is that of a planet moving under the sun's gravitational attraction, as sketched in Figure 1.3.



FIGURE 1.3 A planet moves under the sun's gravitational attraction, a central potential, so its angular momentum is conserved.

Note that the choice of the origin *is* important in this example, because the angular momentum depends upon the location of this reference point.

To calculate the time rate of change of the classical angular momentum, L_c , we need the derivatives

$$\frac{\partial V}{\partial x} = \frac{dV}{dr}\frac{dr}{dx} = \frac{x}{r}\frac{dV}{dr}$$
(1.7)

$$\frac{\partial V}{\partial y} = \frac{dV}{dr}\frac{dr}{dy} = \frac{y}{r}\frac{dV}{dr}$$
(1.8)

From the angular momentum of a particle moving in the x - y plane,

$$L_c = m(x\dot{y} - y\dot{x}) \tag{1.9}$$

we can readily calculate its time derivative as

$$\dot{L}_{c} = m \left(x \frac{d\dot{y}}{dt} - y \frac{d\dot{x}}{dt} \right) = m \left(-x \frac{\partial V}{\partial y} + y \frac{\partial V}{\partial x} \right) = 0$$
(1.10)

In the second step of (1.10) we used Newton's force law, then we used (1.7) and (1.8) for the potential derivatives. We have found a conservation condition—the conservation of angular momentum. What is the symmetry condition?

If you look at the steps in the derivation of (1.10) you will see that the dependence of V on x and y—with these coordinates having equal footing, for example as they determine r—is the essential step leading to the zero in (1.10). Technically, we have assumed a Euclidean metric for the plane of the motion. Equivalently, if we performed a rotation of the plane about the same axis as the particle angular momentum, then the potential would be unaltered, since distance r rather than vector \mathbf{r} is the variable in V. Thus, the symmetry of rotational invariance of the potential leads to conservation of angular momentum of the particle. Generalization of this result for a particle in two dimensions to the result in three dimensions is suggested in Problem 1.1 and is discussed in Section 2.6 of [Gol80].

1.1.2 Noether's Theorem and Curie's Principle

We now consider two results that help organize one's thinking about symmetry in physical systems. The first, Noether's theorem, relating symmetries to conservation conditions, generalizes our examples in Section 1.1.1. It can be proved for a wide variety of systems, including classical mechanics, Maxwell's formulation of electrodynamics, and many systems (both discrete and continuous) that can be described by Lagrangians. The second result, Curie's principle—relating symmetry in causes to symmetry in effects—is just a principle, not a formal theorem.

Noether in a Nutshell. The examples in Section 1.1.1 of symmetries and their conservation laws illustrate Noether's theorem, which can be stated in nontechnical form as follows:

Noether's theorem. If a system has a continuous symmetry property, then there are corresponding quantities whose values are conserved in time.

Table 1.1 summarizes our examples of Noether's theorem on continuous symmetries and conservation laws. The examples given here can be generalized to classical mechanical systems described by Lagrangians expressed in terms of generalized coordinates. Our three examples in Table 1.1 thereby essentially collapse to a single example with different "coordinates." A proof of Noether's theorem that uses variational principles is provided in Section 2.6 of Goldstein's text on classical mechanics [Gol80]. Section 12.7 of the same text provides a more formal discussion of Noether's theorem for continuous systems and fields. Wigner [Wig27a] made similar derivations for quantum mechanics, which are more fully developed in Section IV.1 of Roman's text on elementary particles [Rom61].

6 SYMMETRY IN PHYSICAL SYSTEMS

TABLE 1.1Examples of continuous symmetries of classical mechanical systems and their corresponding conservation laws, illustrating Noether's theorem.

Continuous symmetry		Conserved quantity
Spatial displacement (translationinvariance)		Linear momentum
Time displacement	\bigcirc	Total energy
Rotation about an axis		Angular momentum

Is there a converse to Noether's theorem? Is it true that if we observe conserved quantities in physical systems that there must be a related symmetry? One can construct counterexamples for special systems, but nowadays the persistent and widespread observation of conserved quantities, especially in subatomic systems, is usually taken to be a signal that there exists an underlying symmetry condition, if only we are able to find it.

Emmy Noether (1882–1935) was a leading mathematician of the early twentieth century, best known for her contributions to mathematics. Like the work of her mentor, Paul Gordan (known to physical scientists through the Clebsch-Gordan coefficients that we introduce in Section 7.2.1), Noether's work provided mathematical substance and depth to the concepts and techniques of physics. One tribute to her life and work is the biography edited by Brewer and Smith [Bre81], while another (written by her nephew) is in Grinstein and Campbell's collection of biographies of women of mathematics [Gri87].

In his essays on symmetry, Wigner—one of the founders of the use of symmetry principles in quantum mechanics and its applications—discusses [Wig67, Chapters 2 and 4] the historical development of ideas about symmetry and conservation laws. We take up this thread again in Section 5.5 when we trace the conceptual development of angular momentum.

Curie's Principle. In the pioneering investigations of piezoelectricity and pyroelectricity that he made with his brother Jacques, Pierre Curie enunciated [Cur94] the following guiding principle related to symmetry:

Curie'sprinciple. The symmetry of an isolated system cannot decrease as the system evolves with time.

In the solid-state physics of crystals this is called *Neumann's principle:* Every point-group symmetry (Section **2.5.4)of** a crystal is exhibited by every physical property of that crystal. Indeed, this is the context in which Curie first applied the

principle. Curie's principle has been generalized by Renaud [Ren35] and is discussed extensively in Section 6.2 of Rosen's primer on symmetries [Ros83].

There is no formal proof of the correctness of this principle, the major reason being that there is no quantifiable definition of the degree of symmetry of a system. However, Curie's principle is a very useful guide when investigating symmetries and their consequences.

Pierre Curie (1859 - 1906) made fundamental discoveries in three areas of physics: piezoelectricity, magnetism (the Curie temperature), and radioactivity. With his wife Marie (1867 - 1934), he discovered the elements polonium (named after her native Poland) and radium, both in 1898. They were awarded a Nobel Prize in 1903 for this work.

1.2 SPATIAL SYMMETRIES

In the following two sections we discuss spatial symmetries, beginning with general considerations in this section, then specializing to rotational symmetries—the subject of this book—in Section 1.3. These discussions and methods prepare us for the treatment of discrete symmetries, emphasizing quantum systems, in Section 1.4.

Geometry and Symmetries. Almost as soon as we encounter geometry, we are drawn to considering geometric symmetry. An overview of the relations between geometry in three dimensions and its symmetries is given in Figure 1.4.



FIGURE 1.4 Overview relating geometric symmetries of three types—reflections, rotations, and translations—to abstract geometry and its origins in the practical geometry used in ancient Egypt.

As an example of the geometry-symmetry connection, in plane geometry equilateral triangles and squares are often visually more appealing than arbitrary triangles and quadrilaterals, while in three dimensions regular polyhedra such as a regular tetrahedron or a cube are usually perceived as more interesting than polyhedra with unbalanced sides. As shown in Section 1.2.2, one reason for this is that such figures can fill space (in two and three dimensions) without leaving voids.

8 SYMMETRY IN PHYSICAL SYSTEMS

Albert Einstein—who did so much to change concepts about space and time provides [Ein54] an interesting discussion about the relation between practical geometry (as used for building the Egyptian pyramids), experience, and the abstraction of geometry to Euclid's system and its extensions that Einstein used in his general theory of relativity.

1.2.1 Reflection Symmetry in Nature

In the world around us we observe many examples of reflection symmetry, or close approximations to it. On the other hand, as one zooms into the microscopic scale from macroscopic through mesoscopic scales, a lack of reflection symmetry often becomes evident. We now introduce some terminology used when discussing reflection symmetry, then we discuss reflection symmetry in nature at the mesoscopic level.

Handedness, Chirality, Helicity. Several terms are used to denote that there is a distinction between left and right. One term is just *handedness*, with an obvious meaning, at least for humans when translated from English into an intelligible language. Figure 1.5 reminds you how mirror reflection is related to handedness.



FIGURE 1.5 Hands reflected in mirrors interchange left and right if the mirror is vertical or if the mirror is horizontal. Note that reflection in two mirrors that are at right angles to each other restores the handedness, since diagonally opposite hands are either both left (top left and bottom right) or both right (top right and bottom left).

The term *chirality* (from the Greek for hand, *cheir*) is used in technical contexts, as in stereochemistry and in some areas of subatomic physics. The root word *chiro* also occurs in *chiropractor*—a physician who uses hands to manipulate (Latin *manus*, hand, as in *manuscript*, a handwritten document). Practitioners of angular momentum theory often use their hands to describe rotations; hence, their *handwaving* (nonrigorous) discussions. Molecules that have opposite handedness are called *enantiomers*, and a mixture having the same proportion of the two enantiomers is called *racemic*.

The term *helicity* (from the same Greek root as *helix*, a spiral) is most often used by physicists when describing the projection of intrinsic spins along the direction of motion, especially in relativistic situations such as for photons. The usual definition of the helicity, h, is

$$h = \mathbf{J} \cdot \hat{\mathbf{p}} \tag{1.11}$$

where **J** is the angular momentum of the particle and $\hat{\mathbf{p}}$ is a unit vector along the direction of motion. Sometimes h/J is used instead.

The problem of communicating with extraterrestrial life having an intelligence compatible with that of humans an indication of which side is to be labeled Left and which Right, but without sending pictures (which might accidentally be reconstructed in reverse) has been called by Martin Gardner the Ozma problem. It is posed in Chapter 18 of his book [Gar90], and a solution in terms of a weak-interaction experiment is given in Chapter 22.

Handedness in Nature. One of the first scientists to recognize the significance of handedness in nature—especially at the microscopic level—was Louis Pasteur (1822–1895), who in 1848 discovered the handedness of tartaric-acid molecules, as sketched in Figure 1.6. His discovery is vividly recounted in the biography of Pasteur written by Dubos [Dub76].



FIGURE 1.6 Handedness of the two enantiomers of tartaric acid discovered by Pasteur, and the right-handed helix of DNA discovered by Crick and Watson.

The culmination of discoveries of handedness in biological systems is that by Crick and Watson, who demonstrated the helical structure of DNA molecules in 1953. In Chapter 12 of his book on ambidexterity in the universe, Gardner [Gar90] gives an interesting presentation of Pasteur's discovery, and in later chapters he discusses asymmetry in biological molecules. An unexplained puzzle, to which we return in Section 1.5, is why creatures on Earth have proteins that are almost exclusively left-handed, whereas DNA molecules contain only right-handed sugars.

10 SYMMETRY IN PHYSICAL SYSTEMS

At the subatomic level, the weak interaction exhibits violation of parity symmetry, for example in nuclear beta decay. This possibility was first suggested by Yang and Lee [Yan56] and verified experimentally by Wu et al. [Wu57].

Throughout this book, as motifs at the head of chapters, we have drawings of helical shells in both left- and right-handed varieties, just as they occur in nature. These shells characterize some aspect of the rotational symmetry and angular momentum topics in the chapter. If you look carefully at the pictures, such as Figure 1.7, you will notice that in addition to the handedness of the shell, there is also another reflection symmetry between pictures. To train yourself to recognize such kinds of symmetry, find out what it is. (Discovery favors the prepared mind.) To understand the geometry of these helices and their symmetries, do Problem 1.2.



FIGURE 1.7 Helical shells of the left- and right-handed variety (left side) and their spatial reflections (right side). (Adapted from *Mathematica* notebook Shell.)

1.2.2 Translation Symmetries; Mosaics and Crystals

Before introducing rotational symmetries, we summarize some essential properties of geometrical symmetries resulting from translations in a plane and in three dimensions. Translations are much simpler than rotations, because (unlike the latter in three dimensions) they commute—that is, their order of application is unimportant. We consider figures whose edges are all the same size and that cover a region of the plane (regular polygons) or of three-dimensional space (regular polyhedra) without leaving space between them. They therefore have translational symmetry for discrete translations by the length of a side.

Mosaics. The regular polygons are those that can cover a plane so that no space is left unfilled, thereby forming a mosaic of tiles. Problem 1.3 leads to the proof that the only regular polygons that tile the plane are the triangle, square, and hexagon, as shown in Figure 1.8.

It is interesting to note that each of these figures has a center of reflection symmetry, whereas the pentagon, intermediate between square and hexagon, does not have such a center. An extensive discussion of fivefold symmetry is given in the monograph edited by Hargittai [Har92], and discussions of mathematical puzzles and problems in tiling are given in Martin's book on polyominoes [Mar91].



FIGURE 1.8 The three regular polygons that can tile the plane. The number of edges of each polygon is E.

Crystals. Now consider the situation in three dimensions. Suppose that we have a regular polyhedron with F faces as shown in Figure 1.9. (A polyhedron is regular if all its faces are the same shape and size.)



FIGURE 1.9 The five regular solids that can fill space without leaving voids. For each solid the number in brackets is the number of polyhedron faces, F. (Adapted from *Mathematica* notebook Polyhedra, which results in irregular edges.)

The appearance of a regular polyhedron will be unchanged by any rotation about the center through a discrete angle $\theta = 2\pi n/F$. Such a polyhedron might describe the filling of a region of space without voids by a crystalline material. The regular solids were described by Plato of Athens (427 – 347 B.C.), so they are often called the Platonic solids. Problem 1.4 leads to the proof that the only regular polyhedra have F = 4, 6, 8, 12, and 20, as shown in Figure 1.9 and summarized in Table 1.2.

Polyhedron	F, faces	V, vertices	E, edges	N, edges at each vertex	S, edges at each face
Tetrahedron	4	4	6	3	3
Hexahedron (cube)	6	8	12	3	4
Octahedron	8	6	12	4	3
Dodecahedron	12	20	30	3	5
Icosahedron	20	12	30	5	3

TABLE 1.2 Geometric properties of the regular polyhedra (Platonic solids).

A truncated icosahedron—with the same geometry as a soccer ball (in America) or football (in Europe)—has a particular interest, since it describes the molecule C_{60} , called buckminsterfullerene or the "buckyball." The mathematics of the buckyball is described in a *Scientific American* article by Chung and Sternberg [Chu93].

Now that we have discussed symmetries and conservation laws for physical systems in Section 1.1, as well as reflection and translation symmetries in this section, we turn to the main topic of this book—rotational symmetries.

1.3 ROTATIONAL SYMMETRIES

In this section we introduce the main geometric ideas and formulas relating to rotational symmetries. One of the most important topics is the distinction between active and passive rotations, which we emphasize and clarify in Section 1.3.1. Here we also introduce Euler's scheme for describing rotations in three dimensions and we derive the matrices that describe active rotations of the coordinates of an object. In Section 1.3.2 we develop our understanding of coordinate systems for rotations by considering rotations of the Earth as seen from a fixed point in space. Finally in this section, we provide in Section 1.3.3 a cameo portrait illustrating connections between different topics in this book.

Is Space Isotropic? To modern ways of thinking about the physical sciences, this is probably a meaningless question. I believe it to be *assumed* that space is isotropic, and you will agree with me upon reflection. In an experiment, if we observe that a phenomenon depends on orientation, we attribute this to the presence of interactions. That is, interactions are those things that give rise to a dependence on direction in space.

This viewpoint is consistent with ideas in general relativity, where "curvature" in space-time is attributed to gravitational interactions in the macroworld. Further, in experiments on fundamental symmetries in the microworld—such as breaking of reflection symmetry measured in parity-violation experiments—space is assumed to be isotropic, so the system may be rotated without changing its intrinsic properties.

When you do experiments, a constant problem is to shield the complete appara-

tus of the measurement from so-called "external" influences. Electromagnetic fields are particularly troublesome in this regard. Indeed, if the results depend on the orientation of the apparatus as a whole, this is taken as a signal that the equipment is not sufficiently shielded, rather than as a sign that space is anisotropic.

Given the assumption of the isotropy of space, the subject of rotation symmetry and angular momentum is about how our description of phenomena change when we break this symmetry by choosing a reference frame with a particular orientation. This idea is sketched in Figure 1.10.



FIGURE 1.10 Space is intrinsically isotropic (left), but this symmetry is broken upon choosing a reference axis (middle) or a reference frame (right).

The subject of angular momentum is about how our description of a system changes when we rotate the system relative to a reference frame in space. By analyzing these changes of description we may learn about the interactions within the system. It is to the study of these rotations that we now turn our attention.

1.3.1 Active and Passive Rotations; Euler Angles

A rotation can be considered from one of two viewpoints, active or passive. We now discuss this idea and develop some technical vocabulary and mathematics.

Active Rotations. The first point of view for rotations is called an *active* rotation. Here the observer is in a fixed reference frame while the object—a body in classical mechanics, a field component (\mathbf{E} , \mathbf{B} , or \mathbf{A}) in electromagnetism, or an operator in quantum mechanics—rotates with respect to this reference frame. Such dynamical rotations of objects and transformations of operators are the same as those in classical mechanics. An alternative name for an active rotation is *alibi* (from the Latin for "elsewhere"). In quantum mechanics active rotations are analogous to the Heisenberg viewpoint for time dependence, in which operators are changed by transformations while state vectors (wave functions) are unchanged thereby.

In Figure 1.11 the top half shows active rotation of an ellipsoid, with the observer's eye being kept fixed. Active rotations can be specified by describing the relation between coordinates of a representative point of the object before rotation, $\mathbf{r} = (x, y, z)$, and after rotation, $\mathbf{r}'_A = (x', y', z')$. Geometrically, such rotations are described as indicated in Figure 1.12.



FIGURE 1.11 Active and passive rotations compared. In the top half of the figure an active rotation of the ellipsoid has been made, with the observer's eye fixed. In the bottom half of the figure the ellipsoid is fixed (passive) while the observer's eye rotates around it. Note that the two rotations are the *inverse* of each other.



FIGURE 1.12 Active rotations in terms of the successive rotations through Euler angles α , β , then γ , with the rotations being applied in this order.

An alternative way of describing an active rotation is depicted in Figure 1.13.

Algebra of Active Rotations. Having examined rotations from the geometric viewpoint, it is now time to make an algebraic formulation. Algebraically, in order to describe the active rotation of a representative point on the object, write