# 14

# Hydrogenic Atoms

## Contents

Many physical systems exhibit symmetry. When a symmetry exists it is possible to use Group theory to simplify both the treatment and the understanding of the problem. Central two-body forces, such as the gravitational and Coulomb interactions, give rise to systems exhibiting spherical symmetry (two particles) or broken spherical symmetry (planetary systems). In this Chapter we see how spherical symmetry has been used to probe the details of the hydrogen atom. We find a heirarchy of symmetries and symmetry groups. At the most obvious level is the geometric symmetry group, $SO(3)$, which describes invariance under rotations. At a less obvious level is the dynamical symmetry group, $SO(4)$, which accounts for the degeneracy of the levels in the hydrogen atom with the same principal quantum number. At an even higher level are the spectrum generating groups, $SO(4,1)$ and $SO(4,2)$, which do not maintain energy degeneracy

at all, but rather map any bound (scattering) state of the hydrogen atom into linear combinations of all bound (scattering) states. We begin with a description of the fundamental principles underlying the application of group theory to the study of physical systems. These are the Principle of Relativity (Galileo) and the Principle of Equivalence (Einstein).

## 14.1    Introduction

Applications of group theory in physics start with two very important princples. These are Galileo's Principle of Relativity (of observers) and Einstein's Principle of Equivalence (of states). We show how these principles are used to establish the standard framework for the application of geometric symmetry groups to the treatment of quantum mechanical systems that possess some geometric symmetry. For the hydrogen atom the *geometric symmetry group* is $SO(3)$ and one prediction is that states occur in multiplets with typical angular momentum degeneracy: $2l + 1$. This is seen when we solve the Schrödinger and Klein-Gordon equations for the hydrogen atom — more specifically for the spinless electron in the Coulomb potential of a proton.

Invariance of a Hamiltonian under a group action implies degeneracy of the energy eigenvalues. It is observed that in the nonrelativistic case the energy degeneracy is larger than required by invariance under the rotation group $SO(3)$. If we believe that the greater the symmetry, the greater the degeneracy, we would expect that the Hamiltonian is invariant under a larger group than the geometric symmetry group $SO(3)$. The larger group is called a *dynamical symmetry group*. This group is $SO(4)$ for the hydrogen bound states. It's infinitesimal generators include the components of two three-vectors: the angular momentum vector and the Laplace-Runge-Lenz vector.

When the dynamical symmetry is broken, as in the case of the Klein-Gordon equation, the classical orbit is a precessing ellipse and the bound states with a given principle quantum number $N$ are slightly split according to their orbital angular momentum values $l$.

This suggests that we could look for even larger groups that don't even pretend to preserve (geometric or dynamical) symmetry and do not maintain energy degeneracy. In fact, they map any bound (scattering) state into linear combinations of all other bound (scattering) states. Such groups exist. They are called *spectrum generating groups.* For the hydrogen atom the first spectrum generating group that was discovered was the deSitter group $SO(4, 1)$. A larger spectrum generating group is the conformal group $SO(4, 2)$. We illustrate how spectrum gen-

erating groups have been used to construct eigenfunctions and energy eigenvalues. We also describe how analytic continuations between two qualitatively different types of representations of a noncompact group leads to relations between the bound state spectrum, on the one hand, and the phase shifts of scattering states, on the other.

### 14.2    Two Important Principals of Physics

There are two principles of fundamental importance that allow group theory to be used in profoundly important ways in physics. These are the Principle of Relativity and the Principle of Equivalence. We give a brief statement of both using a variant of Dirac notation.

**Principle of Relativity (of Observers):** Two observers, $S$ and $S'$, describe a physical state $|\psi\rangle$ in their respective coordinate systems. They describe the state by mathematical functions $\langle S|\psi\rangle$ and $\langle S'|\psi\rangle$. The two observers know the relation between their coordinate systems. The mathematical prescription for transforming functions from one coordinate system to the other is $\langle S'|S\rangle$. The set of transformations among observers forms a group. If observer $S'$ wants to determine what observer $S$ has seen, he applies the appropriate transformation, $\langle S|S'\rangle$, to his mathematical functions $\langle S'|\psi\rangle$ to determine how $S$ has described the system:

$$\langle S|\psi\rangle = \langle S|S'\rangle \, \langle S'|\psi\rangle \tag{14.1}$$

The Principle of Relativity of Observers is a statement that *the functions determined by $S'$ in this fashion are exactly the functions used by $S$ to describe the state $|\psi\rangle$.*

**Principle of Equivalence (of States):** Two observes $S$ and $S'$ observe a system, as above. If

- "the rest of the universe"
- "looks the same"

to both $S$ and $S'$, then $S$ can use the mathematical functions $\langle S'|\psi\rangle$ written down by $S'$ to describe a *new* physical state $|\psi'\rangle$

$$\langle S|\psi'\rangle = \langle S'|\psi\rangle \tag{14.2}$$

*and that state must exist.*

In this notation, the transformation of a hamiltonian under a group operation (for example, a rotation in $SO(3)$) is expressed by $\langle S'|H|S'\rangle =$

$\langle S'|S\rangle\langle S|H|S\rangle\langle S|S'\rangle$, the invariance under the transformation $\langle S'|S\rangle$ is represented by $\langle S'|H|S'\rangle = \langle S|H|S\rangle$, and the existence of a $2p_z$ state in a system with spherical symmetry implies the existence (by the Principle of Equivalence) of $2p_x$ and $2p_y$ states, as well as arbitrary linear combinations of these three states.

## 14.3    The Wave Equations

Schrödinger's derivation of a wave equation for a particle of mass $m$ began with the relativistic dispersion relation for the free particle: $p^\mu p_\mu = g_{\mu\nu}p^\mu p^\nu = (mc)^2$. In terms of the energy $E$ and the three-momentum $\mathbf{p}$ this is

$$E^2 - (\mathbf{p}c)^2 = (mc^2)^2 \tag{14.3}$$

Interaction of a particle of charge $q$ with the electromagnetic field is described by the Principle of Minimal Electromagnetic Coupling: $p_\mu \rightarrow \pi_\mu = p_\mu - \frac{q}{c}A_\mu$, where the four-vector potential $A$ consists of the scalar potential $\Phi$ and the vector potential $\mathbf{A}$. These obey $\mathbf{B} = \nabla \times \mathbf{A}$ and $\mathbf{E} = -\nabla\Phi - \frac{1}{c}\frac{\partial\mathbf{A}}{\partial t}$. For an electron $q = -e$, where $e$ is the charge on the proton, positive by convention. In the Coulomb field established by a proton, $\Phi = e/r$ and $\mathbf{A} = \mathbf{0}$, so that $E \rightarrow E + e^2/r$. Here $r$ is the proton-electron distance. The Schrödinger prescription for converting a dispersion relation to a wave equation is to replace $\mathbf{p} \rightarrow (\hbar/i)\nabla$ and allow the resulting equation to act on a spacial function $\psi(\mathbf{x})$. This prescription results in the wave equation

Klein-
Gordon
Equation:
$$\left\{ E^2 - (mc^2)^2 + 2E\left(\frac{e^2}{r}\right) + \left(\frac{e^2}{r}\right)^2 - (-i\hbar c\nabla)^2 \right\} \psi(x) = 0$$

$$\tag{14.4}$$

This equation exhibits spherical symmetry in the sense that it is unchanged (invariant) in form under rotations: $\langle S'|H|S'\rangle = \langle S|H|S\rangle$, where $\langle S'|S\rangle \in SO(3)$. Schrödinger solved this equation, compared its predictions with the spectral energy measurements on the hydrogen atom, was not convinced his theory was any good, and buried this approach in his desk drawer.

Sometime later he reviewed this calculation and took its nonrelativistic limit. Since the binding energy is about 13.6 eV and the electron rest energy $mc^2$ is about $510,000$ eV, it makes sense to write $E = mc^2 + W$, where the principle part of the relativistic energy $E$ is the electron rest

energy and the nonrelativistic energy $W$ is a small perturbation of either ($\simeq 0.0025\%$). Under this substitution, and neglecting terms of order $(W + e^2/r)^2/mc^2$, we obtain the nonrelativistic form of Eq. (14.4):

$$\text{Schrödinger Equation:} \quad \left\{ \frac{\mathbf{p} \cdot \mathbf{p}}{2m} - \frac{e^2}{r} - W \right\} \psi(\mathbf{x}) = \left\{ -\frac{\hbar^2}{2m}\nabla^2 - \frac{e^2}{r} - W \right\} \psi(\mathbf{x}) = 0$$

(14.5)

Eq.(14.4) is now known as the Klein-Gordon equation and its nonrelativistic limit Eq.(14.5) is known as the Schrödinger equation, although the former was derived by Schrödinger before he derived his namesake equation.

**Remark:** Schrödinger began his quest for a theory of atomic physics with Maxwell's Equations, in particular, the eikonal form of these equations. It is no surprise that his theory inherits key characteristics of electromagnetic theory: solutions that are amplitudes, the superposition principle for solutions, and interference effects that come about by squaring amplitudes to obtain intensities. Had he started from classical mechanics, there would be no amplitude-intensity relation and the only superposition principle would have been the superposition of forces or their potentials. The elegant but forced relation between Poisson brackets and commutator brackets ($[A, B]/i\hbar = \{A, B\}$) is an attempt to fit quantum mechanics into the straitjacket of classical mechanics.

## 14.4   Quantization Conditions

The standard approach to solving partial differential equations is to separate variables. Since the two equations derived above have spherical symmetry, it is useful to introduce spherical coordinates: $(r, \theta, \phi)$. In this coordinate system the Laplacian is

$$\nabla^2 = \left( \frac{1}{r}\frac{\partial}{\partial r}r \right)^2 + \frac{\mathcal{L}^2(S^2)}{r^2}$$

(14.6)

$$\mathcal{L}^2(S^2) = \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\,\sin\theta\,\frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}$$

(14.7)

The second order differential operator $\mathcal{L}^2(S^2)$ is the Laplacian on the sphere $S^2$. Its eigenfunctions are the spherical harmonics $Y_m^l(\theta, \phi)$ and its spectrum of eigenvalues is $\mathcal{L}^2(S^2)Y_m^l(\theta, \phi) = -l(l+1)Y_m^l(\theta, \phi)$. The integers $(l, m)$ satisfy $l = 0, 1, 2, \cdots$ and $-l \leq m \leq +l$. The negative sign and discrete spectrum characteristically indicate that $S^2$ is compact.

The partial differential equations Eqs.(14.4) and (14.5) are reduced to ordinary differential equations by substituting the ansatz

$$\psi(r, \theta, \phi) \rightarrow \frac{1}{r} R(r) Y_m^l(\theta, \phi) \tag{14.8}$$

into these equations, replacing the angular part of the Laplacian by the eigenvalue $-l(l+1)$, and multiplying by $r$ on the left. This gives the simple second order ordinary differential equation

$$\left( \frac{d^2}{dr^2} + \frac{A}{r^2} + \frac{B}{r} + C \right) R(r) = 0 \tag{14.9}$$

The values of the coefficients $A, B, C$ that are obtained for the Klein-Gordon equation and the Schrödinger equation are

| Equation | $A$ | $B$ | $C$ |
|---|---|---|---|
| Klein-Gordon | $-l(l+1) + (e^2/\hbar c)^2$ | $2Ee^2/(\hbar c)^2$ | $\left[ E^2 - (mc^2)^2 \right]/(\hbar c)^2$ |
| Schrödinger | $-l(l+1)$ | $2me^2/\hbar^2$ | $2mW/\hbar^2$ |

$$\tag{14.10}$$

There is a standard procedure for solving simple ordinary differential equations of the type presented in Eq.(14.9). This is the Frobenius method. The steps involved in this method, and the result of each step, are summarized in Table 14.1.

The energy eigenvalues for the bound states of both the relativistic and nonrelativistic problems are expressed in terms of the radial quantum number $n = 0, 1, 2, \cdots$ and the angular momentum quantum number $l = 0, 1, 2, \cdots$, mass $m$ of the electron, or more precisely the reduced mass of the proton-electron pair $m_{red}^{-1} = m_e^{-1} + M_p^{-1}$, and the fine structure constant [23]

$$\alpha = \frac{e^2}{\hbar c} = \frac{1}{137.035\ 999\ \underline{796}(70)} = 0.007\ 297\ 352\ 53\underline{1\ 3}(3\ 8) \tag{14.11}$$

This is a dimensionless ratio of three physical constants that are fundamental in three "different" areas of physics: $e$ (electromagnetism), $\hbar$ (quantum mechanics), and $c$ (relativity). It is one of the most precisely measured of the physical constants. The bound state energy eigenvalues are

Table 14.1. *Left column lists the steps followed in the Frobenius method for finding the square-integrable solutions of simple ordinary differential equations. Right column shows the result of applying the step to Eq.(14.9).*

| | Procedure | Result |
|---|---|---|
| 1 | Locate singularities | $0, \infty$ |
| 2 | Determine analytic behavior at singular points | $r \to 0 : R \simeq r^\gamma, \quad \gamma(\gamma - 1) + A = 0$ <br> $r \to \infty : R \simeq e^{\lambda r}, \quad \lambda^2 + C = 0$ |
| 3 | Keep only $\mathcal{L}^2$ solutions | $\gamma = \frac{1}{2} + \sqrt{(\frac{1}{2})^2 - A}, \quad \lambda = -\sqrt{-C}$ |
| 4 | Look for solutions with proper asymptotic behavior | $R = r^\gamma e^{\lambda r} f(r)$ |
| 5 | Construct DE for $f(r)$ | $\left[ (rD^2 + 2\gamma D) + (2\lambda\gamma + B + 2\lambda rD) \right] f(r) = 0$ |
| 6 | Construct recursion relation | $f_{j+1} = -\frac{2\lambda(j+\gamma)+B}{j(j+1)+2\gamma(j+1)} \, f_j$ |
| 7 | Look at asymptotic behavior | $f \simeq e^{-2\lambda r}$ if series doesn't terminate <br> $\simeq e^{+1\lambda r}$ if series does terminate $(\lambda < 0)$ |
| 8 | Construct quantization condition | $2\lambda(n + \gamma) + B = 0$ or <br> $n + \dfrac{1}{2} + \sqrt{(\dfrac{1}{2})^2 - A} = \dfrac{B}{2\sqrt{-C}}$ |
| 9 | Construct explicit solutions | $E = \dfrac{mc^2}{\sqrt{1+(\alpha/N')^2}} \qquad W = -\frac{1}{2}mc^2\alpha^2 \, \frac{1}{N^2}$ <br> $N' = n + \frac{1}{2} + \sqrt{(l+\frac{1}{2})^2 - \alpha^2} \quad N = n + l + 1$ |

<div align="center">

Klein-Gordon Equation        Schrödinger Equation

</div>

$$E(n,l) \;\;=\;\; \frac{mc^2}{\sqrt{1 + (\alpha/N')^2}} \qquad\qquad W(n,l) \;\;=\;\; -\frac{1}{2}mc^2\alpha^2\frac{1}{N^2}$$

$$N' \;\;=\;\; n + \frac{1}{2} + \sqrt{\left(l + \frac{1}{2}\right)^2 - \alpha^2} \qquad\qquad N \;\;=\;\; n + l + 1$$

$$(14.12)$$

Both the nonrelativistic and relativistic energies have been plotted in Fig. 14.1. The nonrelativistic energies for the hydrogen atom appear as the darker lines. The nonrelativistic energy has been normalized by dividing by the hydrogen atom ground state energy $|W_1| = \frac{1}{2}mc^2\alpha^2$. These normalized energy levels decrease to zero like $1/N^2$, where $N = n+l+1$ is the principle quantum number. The energies are displayed as a function of the orbital angular momentum $l$. The relativistic energies of the

# Energy Eigenvalues, H Atom
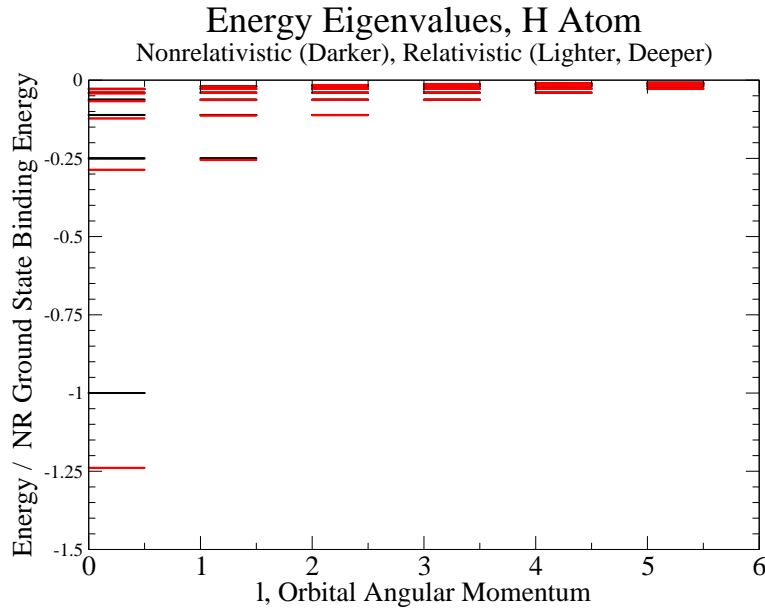## Nonrelativistic (Darker), Relativistic (Lighter, Deeper)



Fig. 14.1. Spectrum of the hydrogen atom, normalized by the energy of the nonrelativistic ground state. The nonrelativistic spectrum is darker. The relativistic spectrum has been computed for $Z = 50$. These energies are computed by replacing $\alpha \to Z\alpha$ everywhere.

bound states for the proton-electron system converge to the rest energy $mc^2$ as $N'$ increases. When this limit is removed these energies (also rescaled by dividing by $\frac{1}{2}mc^2\alpha^2$) can be plotted on the same graph. At the resolution shown, the two sets of rescaled energies are indistinguishable. To illustrate the difference, we have instead computed and plotted the bound state spectrum for a single electron in a potential with positive charge $Z$. The energies in this case are obtained by the substitution $\alpha \to Z\alpha$ everywhere. The energies of these bound states have been renormalized by subtracting the limit $mc^2$ and dividing by the nonrelativistic energy for the same ion: $\frac{1}{2}mc^2(Z\alpha)^2$. The energy difference between the $1s$ ground states is pronounced; this difference decreases rapidly as the principle qunatum number increases.

## 14.5    Geometric Symmetry $SO(3)$

Symmetry implies degeneracy.

To see this, assume $g_i \in G$ are group operations that leave a hamiltonian $H$ invariant (unchanged in form)

$$g_i H g_i^{-1} = H \quad \text{or} \quad g_i H = H g_i \tag{14.13}$$

When $G$ is a group of geometric transformations the physical interpretation of this equation is as follows. The hamiltonian $H$ has the same form in two coordinate systems that differ by the group operation $g_i$. Under this condition, if $|\psi\rangle$ is an eigenstate of $H$ with eigenvalue $E$, then $g_i|\psi\rangle$ is also an eigenstate of $H$ with the same energy eigenvalue $E$. The demonstration is straightforward:

$$H(g_i|\psi\rangle) = (Hg_i)|\psi\rangle = (g_iH)|\psi\rangle = g_i(H|\psi\rangle) = g_i(E|\psi\rangle) = E(g_i|\psi\rangle) \tag{14.14}$$

To illustrate this idea, assume that $|\psi\rangle = \psi_{2p_z}(\mathbf{x})$. A rotation by $\pi/2$ radians about the $y$-axis maps this state to $\psi_{2p_x}(\mathbf{x})$ and a rotation by $\pi/2$ radians about the $x$-axis maps this state to $-\psi_{2p_y}(\mathbf{x})$. By invariance (of the hamiltonian) under the rotation group and the Principle of Equivalence, these new functions describe possible states of the system, and these states must exist.

The rotation group $O(3)$ leaves the hamiltonian of the hydrogen atom invariant in both the nonrelativistic and relativistic cases. In the nonrelativistic case, $H = \frac{\mathbf{p} \cdot \mathbf{p}}{2m} - \frac{e^2}{r}$. The scalar $\mathbf{p} \cdot \mathbf{p} = -\hbar^2 \nabla^2$ is invariant under rotations, as is also the potential energy term $-e^2/r$. Rotation operators can be expressed in terms of the infinitesimal generators of rotations about axis $i$: $\epsilon_{ijk}x_j\partial_k$. These geometric operators are proportional to the physical angular momentum operators $\mathbf{L}_i = (\mathbf{r} \times \mathbf{p})_i = (\hbar/i)\epsilon_{ijk}x_j\partial_k$. Finite rotations can be expressed as exponentials as follows:

$$R(\theta) = e^{\epsilon_{ijk}\theta_i x_j \partial_k} = e^{i\theta \cdot \mathbf{L}/\hbar} \tag{14.15}$$

The angular momentum operators $\mathbf{L} = \mathbf{r} \times \mathbf{p}$ share the same commutation relations as the infinitesimal generators of rotations $\mathbf{r} \times \nabla$, up to the proportionality factor $\hbar/i$. The commutation relations are

$$[L_i, L_j] = i\hbar\epsilon_{ijk}L_k \tag{14.16}$$

It is useful to construct linear combinations of these operators that have canonical commutation relations of the type described in Chapter 10.

To this end we define the raising $(L_+)$ and lowering $(L_-)$ operators by $L_\pm = L_x \pm iL_y$. The commutation relations are

$$
\begin{aligned}
[L_z, L_\pm] &= \pm\hbar L_\pm & (14.17) \\
[L_+, L_-] &= 2\hbar L_z & (14.18)
\end{aligned}
$$

These angular momentum operators are related to the two boson operators as follows: $L_z = \hbar\frac{1}{2}(a_1^\dagger a_1 - a_2^\dagger a_2)$ $L_+ = \hbar a_1^\dagger a_2$, $L_- = \hbar a_2^\dagger a_1$. As a result, the angular momentum operators have matrix representations with basis vectors $|\ n_1 \quad n_2\ \rangle = |\ {}^{\ j}_{\ m}\ \rangle$, with $n_1 = 0, 1, 2, \ldots$, $n_2 = 0, 1, 2, \ldots$, $n_1 + n_2 = 2j$, $n_1 - n_2 = 2m$, $-j \le m \le +j$. These basis vectors describe the finite dimensional irreducible representations of the covering group $SU(2)$ of $SO(3)$. The subset of representations with $j = l$ (integer) describes representations of $SO(3)$.

To see this we construct a coordinate representation of the angular momentum operators. In spherical coordinates $((x, y, z) \to (r, \theta, \phi)$ with $x = r\sin\theta\cos\phi)$ these operators are

$$
\begin{aligned}
L_z &= \frac{\hbar}{i}\frac{\partial}{\partial\phi} \\
L_\pm &= \hbar\left(\pm\frac{\partial}{\partial\theta} + i\,\frac{\cos\theta}{\sin\theta}\frac{\partial}{\partial\phi}\right)
\end{aligned}
\qquad (14.19)
$$

The functions on $R^3$ that transform under the angular momentum operators can be constructed from the mixed basis argument:

$$
\langle\theta\phi|L_-|\ {}^{\ l}_{\ m}\ \rangle
$$

$$
\downarrow \qquad\qquad\qquad \downarrow \qquad\qquad (14.20)
$$

$$
\langle\theta\phi|L_-|\theta'\phi'\rangle\,\langle\theta'\phi'|\ {}^{\ l}_{\ m}\ \rangle = \langle\theta\phi|\ {}^{\ l'}_{\ m'}\ \rangle\langle\ {}^{\ l'}_{\ m'}\ |L_-|\ {}^{\ l}_{\ m}\ \rangle
$$

As usual, the intermediate arguments (with primes) are dummy arguments that are summed or integrated over. The symbols in Eq.(14.20) have the following meaning

$\langle\theta\phi|L_-|\theta'\phi'\rangle$      Matrix element of the angular momentum shift down oper-
ator in the coordinate representation: $\hbar\left(-\frac{\partial}{\partial\theta}+i\frac{\cos\theta}{\sin\theta}\frac{\partial}{\partial\phi}\right)$
$\delta(\cos\theta'-\cos\theta)\delta(\phi'-\phi)$.

$\langle\,{}^{l'}_{m'}\,|L_-|\,{}^{l}_{m}\,\rangle$      Matrix element of the angular momentum shift down oper-
ator in the algebraic representation: $\hbar\sqrt{(l'-m')(l+m)}$
$\delta_{l'l}\,\delta_{m',m-1}$.

$\langle\theta\phi|\,{}^{l}_{m}\,\rangle$      Matrix element of the similarity transformation between the
coordinate representation and algebraic representation. Also
called spherical harmonic: $Y^l_m(\theta,\phi)$.

This relation can be used to show that there are no geometric functions
associated with values of the quantum number $j$ that are half integral.
It can also be used to constuct the extremal function $Y^l_{-l}(\theta,\phi)$ by solving
the equation $L_-Y^l_{-l}(\theta,\phi)=0$ in the coordinate representation (Problem
14.12). Finally, the action of the shift up operators can be used to
constuct the remaining functions $Y^l_m(\theta,\phi)$ through the recursion relation
involving both the coordinate and the algebraic representations of the
shift up operator $L_+$

$$L_+Y^l_m(\theta,\phi)=Y^l_{m+1}(\theta,\phi)\sqrt{(l-m)(l+m+1)} \qquad (14.21)$$

The lowest spherical harmonics ($l=0,1,2,3$) are collected in Table 14.2.

Table 14.2. *Spherical harmonics* $Y^l_m(\theta,\phi)$ *for low values of $l$ and $m$.*

| $m$ | $l=0$ | $l=1$ | $l=2$ | $l=3$ |
|---|---|---|---|---|
| 0 | $\sqrt{\frac{1}{4\pi}}$ | $\sqrt{\frac{3}{4\pi}}\cos\theta$ | $\sqrt{\frac{5}{16\pi}}(3\cos^2\theta-1)$ | $\sqrt{\frac{7}{16\pi}}(5\cos^3\theta-3\cos\theta)$ |
| $\pm1$ | | $\mp\sqrt{\frac{3}{8\pi}}\sin\theta\,e^{\pm i\phi}$ | $\mp\sqrt{\frac{15}{8\pi}}\cos\theta\sin\theta\,e^{\pm i\phi}$ | $\mp\sqrt{\frac{21}{64\pi}}\sin\theta(5\cos^2\theta-1)\,e^{\pm i\phi}$ |
| $\pm2$ | | | $\sqrt{\frac{15}{32\pi}}\sin^2\theta\,e^{\pm 2i\phi}$ | $\sqrt{\frac{105}{32\pi}}\sin^2\theta\cos\theta\,e^{\pm 2i\phi}$ |
| $\pm3$ | | | | $\mp\sqrt{\frac{35}{64\pi}}\sin^3\theta\,e^{\pm 3i\phi}$ |

**Remark:** The spectrum of the Casimir invariant for the rotation
group $SO(3)$, or more specifically the Laplace-Beltrami operator con-
structed from its infinitesimal generators acting on the sphere parame-
terized by coordinates $(\theta,\phi)$, is $-l(l+1)$, $l=0,1,2,\ldots$. The fact that
the spectrum is negative means that the space, $S^2$, on which these oper-
ators act, is compact. By the same token, the spectrum of the square of

the angular momentum operator, $\mathbf{L} \cdot \mathbf{L}$, is $\hbar^2 l(l+1)$. This means physically that the inner product of the angular momentum operator with itself is never negative, and is quantized by integer angular momentum values, measured in units of Planck's constant $\hbar$.

## 14.6   Dynamical Symmetry $SO(4)$

Symmetry implies degeneracy.

The greater the symmetry, the greater the degeneracy.

The states of the nonrelativistic hydrogen atom with fixed principal quantum number $N = n + l + 1$ are degenerate, with energy $E_N = -\frac{1}{2}mc^2\alpha^2\frac{1}{N^2}$. There are $\sum_{l=0}^{l=N-1}(2l+1) = N^2$ states with this energy. This $N^2$-fold degeneracy is larger than the $2l+1$-fold degeneracy required by rotational invariance of the hamiltonian. If we believe the converse, that degeneracy implies symmetry, then we might be led to expect that the hydrogen atom exhibits more symmetry than meets the eye.

In fact this symmetry, called a dynamical symmetry [61], exists and is related to a constant of motion that is peculiar to $1/r^2$ force laws. This constant of motion is known as the Laplace-Runge-Lenz vector. It is a constant of unperturbed planetary motion, for which the force law has the form $\frac{d\mathbf{p}}{dt} = -K\frac{\mathbf{r}}{r^3}$, where $K = GMm$, $G$ is the universal gravitational constant, $M$ and $m$ are the two attracting masses, and $\mathbf{r} = x\hat{\mathbf{i}} + y\hat{\mathbf{j}} + z\hat{\mathbf{k}}$ is the vector from one mass to the other. The time derivative of the vector $\mathbf{p} \times \mathbf{L}$ is

$$
\begin{aligned}
\frac{d}{dt}\left(\mathbf{p} \times \mathbf{L}\right) &= \frac{d\mathbf{p}}{dt} \times \mathbf{L} + \mathbf{p} \times \frac{d\mathbf{L}}{dt} \\
&\qquad\qquad \downarrow \qquad\qquad\qquad \downarrow \\
&= -K\frac{\mathbf{r}}{r^3} \times (\mathbf{r} \times m\dot{\mathbf{r}}) + 0 \qquad (14.22) \\
&= -mK\frac{\mathbf{r}(\mathbf{r} \cdot \dot{\mathbf{r}}) - \dot{\mathbf{r}}(\mathbf{r} \cdot \mathbf{r})}{r^3} = mK\frac{d}{dt}\left(\frac{\mathbf{r}}{r}\right)
\end{aligned}
$$

In going from the first line in Eq. (14.22) to the second, we use the fact that $\mathbf{L}$ is a constant of motion in any spherically symmetric potential. We also use the force law for a $1/r$ potential. In going from the second line to the third, we express the cross product $\mathbf{r} \times \mathbf{L}$ in terms of (generally) nonparallel vectors $\mathbf{r}$ and $\dot{\mathbf{r}}$. We also use the identity $\frac{d}{dt}\frac{\mathbf{r}}{r} = \dot{\mathbf{r}}/r - (\dot{\mathbf{r}} \cdot \mathbf{r})\,\mathbf{r}/r^3$. The result is that the Laplace-Runge-Lenz vector $\mathbf{M}$ is a constant of motion: $d\mathbf{M}/dt = 0$, where

$$\mathbf{M} = \frac{\mathbf{p} \times \mathbf{L}}{m} - K\frac{\mathbf{r}}{r} \tag{14.23}$$

In the transition from classical to quantum mechanics the operator obtained from the classical operator in Eq. (14.23) is not hermitian. Pauli [56] symmetrized it properly, defining the hermitian quantum mechanical operator

$$\hat{\mathbf{M}} = \frac{\hat{\mathbf{p}} \times \hat{\mathbf{L}} - \hat{\mathbf{L}} \times \hat{\mathbf{p}}}{2m} - K\frac{\hat{\mathbf{r}}}{r} \tag{14.24}$$

where the ˆ over the classical symbol indicates a quantum mechanical operator. We will dispense with the ˆ over operators, in part to simplify notation, in part to prevent uncertainties in interpretation of the operator **r**.

The hermitian operator **M** in Eq. (14.23) is a constant of motion, as it commutes with the nonrelativistic hamiltonian: $[H, \mathbf{M}] = 0$. The six operators $L_i, M_j$ obey the following commutation relations

$$\begin{aligned}
[L_i, L_j] &= i\hbar\epsilon_{ijk}\, L_k \\
[L_i, M_j] &= i\hbar\epsilon_{ijk}\, M_k \\
[M_i, M_j] &= \left(-\frac{2H}{m}\right) i\hbar\epsilon_{ijk}\, L_k
\end{aligned} \tag{14.25}$$

These are the commutation relations for the Lie algebra of the group $SO(4)$ for bound states ($E < 0$) or $SO(3,1)$ for excited states ($E > 0$). The operators **L** and **M** also obey

$$\begin{aligned}
\mathbf{L} \cdot \mathbf{M} = \mathbf{M} \cdot \mathbf{L} &= 0 \\
\\
\mathbf{M} \cdot \mathbf{M} &= \frac{2H}{m}\left(\mathbf{L} \cdot \mathbf{L} + \hbar^2\right) + K^2
\end{aligned} \tag{14.26}$$

In order to simplify the discussion to follow, and make this discussion as independent of the principal quantum number $N$ as possible, we renormalize the Laplace-Runge-Lenz vector by a scale factor as follows: $\mathbf{M}' = \left(-\frac{m}{2H}\right)^{1/2}\mathbf{M}$. (For $E > 0$ change $- \rightarrow +$ and $SO(4) \rightarrow SO(3,1)$.) The commutation relations of these operators are now

$$\begin{aligned}
[L_i, L_j] &= i\hbar\epsilon_{ijk}\, L_k \\
\left[L_i, M_j'\right] &= i\hbar\epsilon_{ijk}\, M_k' \\
\left[M_i', M_j'\right] &= i\hbar\epsilon_{ijk}\, L_k
\end{aligned} \tag{14.27}$$

The Lie algebra $\mathfrak{so}(4)$ is the direct sum of two Lie algebras of type $\mathfrak{so}(3)$ (cf. Figs. 10.3, 10.8($b$)). It is useful to introduce two vector operators $\mathbf{A}$ and $\mathbf{B}$ as follows

$$\mathbf{A} = \tfrac{1}{2}(\mathbf{L} + \mathbf{M}')$$

$$\mathbf{B} = \tfrac{1}{2}(\mathbf{L} - \mathbf{M}')$$

(14.28)

The operators $\mathbf{A}$ and $\mathbf{B}$ have angular momentum commutation relations. Further, they mutually commute. Finally, their squares have the same spectrum.

It is useful at this point to introduce the Schwinger representation for the angular momentum operators $\mathbf{A}$ in terms of two independent boson modes: $A_3 = \tfrac{1}{2}(a_1^\dagger a_1 - a_2^\dagger a_2), A_+ = a_1^\dagger a_2, A_- = a_2^\dagger a_1$ (for simplicity, set $\hbar \to 1$). A similar representation of the angular momentum operators $\mathbf{B}$ in terms of two independent boson operators $b_1, b_2$ and their creation operators is also introduced.

Basis states for a representation of the algebra spanned by the operators $\mathbf{A}$ have the form $|p_1, p_2\rangle$, with $p_1 + p_2 = 2j_a$ constant and $p_1 - p_2 = m_a$. The $2j_a + 1$ basis states correspond to $p_1 = 2j_a, p_2 = 0$; $p_1 = 2j_a - 1, p_2 = 1$; etc. For $\mathbf{B}$ the basis states are $|q_1, q_2\rangle$, with $q_1 + q_2 = 2j_b$ constant and $q_1 - q_2 = m_b$. The invariant operators are $\mathbf{A} \cdot \mathbf{A} = j_a(j_a+1)$ and $\mathbf{B} \cdot \mathbf{B} = j_b(j_b+1)$. Since $\mathbf{A} \cdot \mathbf{A} = \mathbf{B} \cdot \mathbf{B}$ (cf. Problem 14.15), $j_a = j_b$ and the set of states related by the shift operators is $(2j+1)^2$ fold degenerate, where $2j+1 = N = n + l + 1$.

States with good $l$ and $m$ quantum numbers can be constructed from these states using Clebsch-Gordon coefficients:

$$| \begin{matrix} l \\ m \end{matrix} \rangle = | \begin{matrix} j/2 & j/2 \\ m_a & m_b \end{matrix} \rangle \langle \begin{matrix} j/2 & j/2 \\ m_a & m_b \end{matrix} | \begin{matrix} l \\ m \end{matrix} \rangle$$

(14.29)

The action of the Laplace-Runge-Lenz shift operators on these states, and the spherical harmonics, is determined in a straightforward way. For example, $M'_+ = A_+ - B_+ = a_1^\dagger a_2 - b_1^\dagger b_2$, so that

$$M'_+ Y_m^l = \langle \theta\phi| \left( | \begin{matrix} j/2 & j/2 \\ m_a + 1 & m_b \end{matrix} \rangle \langle \begin{matrix} j/2 & j/2 \\ m_a & m_b \end{matrix} | \begin{matrix} l \\ m \end{matrix} \rangle \times \sqrt{(j/2 - m_a)(j/2 + m_a + 1)} \right. -$$

$$\left. | \begin{matrix} j/2 & j/2 \\ m_a & m_b + 1 \end{matrix} \rangle \langle \begin{matrix} j/2 & j/2 \\ m_a & m_b \end{matrix} | \begin{matrix} l \\ m \end{matrix} \rangle \times \sqrt{(j/2 - m_b)(j/2 + m_b + 1)} \right)$$

(14.30)

In general, the Laplace-Runge-Lenz operators shift the values of $l$ and $m$ by $\pm 1$ or $0$, while the angular momentum shift operators change only $m$ by $\pm 1$. However, for certain stretched values of the Clebsch-Gordon coefficients, the Laplace-Runge-Lenz vectors act more simply, for example [15]

$$M'_z |N \begin{smallmatrix} l \\ \pm l \end{smallmatrix} \rangle = D_1 |N \begin{smallmatrix} l+1 \\ \pm l \end{smallmatrix} \rangle \qquad D_1 = \frac{1}{N}\sqrt{\frac{N^2-(l+1)^2}{2l+3}}$$

$$M'_\pm |N \begin{smallmatrix} l \\ \pm l \end{smallmatrix} \rangle = \pm D_2 |N \begin{smallmatrix} l+1 \\ \pm(l+1) \end{smallmatrix} \rangle \qquad D_2 = \frac{1}{N}\sqrt{\frac{2l+2}{2l+3}[N^2-(l+1)^2]}$$

$$(14.31)$$

## 14.7    Relation With Dynamics in Four Dimensions

The operators $\mathbf{L}$ and $\mathbf{M}'$ are infinitesimal generators for the orthogonal group $SO(4)$. The relation between motion in the presence of a Coulomb or gravitational potential and motion in four (mathematical) dimensions was clarified by Fock [19]. Motion of a particle in a $1/r$ potential is equivalent to motion of a free particle in the sphere $S^3 \subset R^4$.

It is useful first to establish an orthogonal coordinate system in $R^3$. It is natural to do this in terms of the constant physical vectors that are available. These include the vectors $\mathbf{L}$ and $\mathbf{M}$. Their cross product $\mathbf{W} = \mathbf{L} \times \mathbf{M}$ is orthogonal to both and also a constant of motion. These classical vectors obey:

$$
\begin{aligned}
\mathbf{L} &= \mathbf{r} \times \mathbf{p} & \mathbf{L} \cdot \mathbf{L} &= L^2 \\
\mathbf{M} &= \frac{\mathbf{p} \times \mathbf{L}}{m} - K\frac{\mathbf{r}}{r} & \mathbf{M} \cdot \mathbf{M} &= M^2 = \frac{2E}{m}L^2 + K^2 \\
\mathbf{W} &= \frac{\mathbf{p}}{m}L^2 - K\frac{\mathbf{L} \times \mathbf{r}}{r} & \mathbf{W} \cdot \mathbf{W} &= L^2 M^2
\end{aligned}
$$

$$(14.32)$$

The particle moves in a plane perpendicular to the angular momentum vector $\mathbf{L}$, since $\mathbf{r} \cdot \mathbf{L} = 0$. The momentum vector moves in the same plane, since $\mathbf{p} \cdot \mathbf{L} = 0$. While $\mathbf{r}$ moves in an ellipse, the momentum vector moves on a circle. For simplicity we choose the $z$ axis in the direction of $\mathbf{L}$ and the $x$- and $y$-axes in the directions of $\mathbf{M}$ and $\mathbf{W}$. In this coordinate system $p_z = 0$, $p_x = \mathbf{p} \cdot \mathbf{M}/\sqrt{\mathbf{M} \cdot \mathbf{M}}$ and $p_y = \mathbf{p} \cdot \mathbf{W}/\sqrt{\mathbf{W} \cdot \mathbf{W}}$. The two nonzero components of the momentum vector are not independent,

but obey the constraint

$$p_x^2 + \left(p_y - \frac{mM}{L}\right)^2 = \left(\frac{mK}{L}\right)^2 \qquad (14.33)$$

This is the equation of a circle in the plane containing the motion. As the particle moves in the plane of motion on an elliptical orbit with one focus at the source, its momentum moves in the same plane on a circular orbit (radius $mK/L$) with the center displaced from the origin by $mM/L$.

The circle in $R^3$ is lifted to a circle in $S^3 \subset R^4$ by a projective transformation. We extend coordinates from $R^3$ to $R^4$ as follows:

$$\begin{aligned}(x, y, z) \in R^3 &\rightarrow (w, x, y, z) \in R^4 \\ (p_x, p_y, p_z) \in R^3 &\rightarrow (p_w, p_x, p_y, p_z) \in R^4\end{aligned} \qquad (14.34)$$

With $p_0 = \sqrt{-2E/m}$, define the unit vector $\hat{\mathbf{u}} \in S^3 \subset R^4$ by the projective transformation $T$:

$$\hat{\mathbf{u}} \overset{T}{=} \frac{\mathbf{p} \cdot \mathbf{p} - p_0^2}{\mathbf{p} \cdot \mathbf{p} + p_0^2} \, \hat{\mathbf{w}} + \frac{2p_0}{\mathbf{p} \cdot \mathbf{p} + p_0^2} \, \mathbf{p} \qquad (14.35)$$

Here $\hat{\mathbf{w}}$ is a unit vector in $R^4$ that is orthogonal to all vectors in the physical space $R^3$. The transformation in [Eq.(14.35)] is a stereographic projection. It is invertible and preserves angles (conformal). It is a simple matter to check that $\hat{\mathbf{u}}$ is a unit vector. The circular trajectory in $R^3$ [Eq.(14.33)] lifts to a circle in $S^3$. Reversibly, circles in $S^3$ project down to circles in the physical $R^3$ space under the reverse transformation.

Rotations in $SO(4)$ rigidly rotate the sphere $S^3$ into itself. They rotate circles into circles, which then project down to circular momentum trajectories in the physical space $R^3$:

$$\text{circle in } R^3 \overset{T}{\longrightarrow} \text{circle in } S^3 \overset{SO(4)}{\longrightarrow} \text{circle in } S^3 \overset{T^{-1}}{\longrightarrow} \text{circle in } R^3 \quad (14.36)$$

The subgroup $SO(3)$ of rotations around the $\hat{\mathbf{w}}$ axis acts only the the physical space $R^3$. In this subgroup, the subgroup $SO(2)$ of rotations around the $\mathbf{L}$ axis leaves $\mathbf{L}$ fixed and simply rotates $\mathbf{M}$ in the plane of motion. The coset representatives $SO(3)/SO(2)$ act to reorient the plane of motion by rotating the angular momentum vector $\mathbf{L}$ while keeping the magnitude of $\mathbf{M}$ fixed. Rotations in the coset $SO(4)/SO(3)$ act to change the lengths of both $\mathbf{L}$ and $\mathbf{M}$. All group operations in $SO(4)$ keep $p_0$ fixed. In this way the group $SO(4)$ maps states with principal quantum number $N$ into (linear combinations of) states with the same

principal quantum number $N$. In short, $SO(4)$ acts on the bound hydrogen atom states through unitary irreducible representations of dimension $N^2 = (n + l + 1)^2$.

## 14.8  DeSitter Symmetry $SO(4,1)$

The dynamical symmetry group $SO(4)$ that rotates bound states to bound states does not change their energy; the dynamical symmetry group $SO(3,1)$ that rotates scattering states to scattering states does not change their energy either. It would be nice to find a set of transformations that rescales the energy. If such a group could be found, it would be possible, for example, to map the $1s$ ground state into any other bound state. Such a group exists: it is the deSitter group $SO(4,1)$ [51,54].

That such a group might exist is strongly suggested by the appearance of the hydrogen atom spectrum, as replotted in Fig. 14.2. In this figure we have multiplied each energy eigenvalue by $-N^3$, where $N$ is the principle quantum number. The rescaled energies have been plotted as a function of $N$ (vertically) and orbital angular momentum quantum number $l$ (horizontally). In this format, the ewigenvalue spectrum bears a strong resemblance to the spectrum of states that supports finite-dimensional representations of $\mathfrak{su}(2)$ (Fig. 6.1) and the infinite-dimensional representations of $\mathfrak{su}(1,1)$ (Fig. 11.2).

We begin with a group that preserves inner products in some $N$-dimensional linear vector space: $\mathbf{x}' = M\mathbf{x}$, with $M$ a transformation in the group and the inner product defined by $(\mathbf{x}, \mathbf{x})_N = \mathbf{x}^t \mathbf{g} \mathbf{x} = x_i g_{ij} x_j$. As always, the metric-preserving condition leads to $M^t G M = G$.

It is useful to define a new $N$-vector $\mathbf{y}$ as a scaled version of the original vector: $\mathbf{y} = \lambda \mathbf{x}$. We introduce two additional coordinates by defining $z_1 = \lambda$ and $z_2 = \lambda(\mathbf{x}, \mathbf{x})_N$. With these definitions we find the conformal condition

$$(\mathbf{y}, \mathbf{y})_N - z_1 z_2 = (\lambda \mathbf{x}, \lambda \mathbf{x})_N - \lambda \left[ \lambda(\lambda \mathbf{x}, \lambda \mathbf{x})_N \right] = 0 \qquad (14.37)$$

The conformal condition defines an inner product in the $N + 2$ dimensional linear vector space that is nondiagonal in the coordinates $\mathbf{y}, z_1, z_2$ but diagonal in the coordinates $\mathbf{y}, y_{N+1}, y_{N+2}$, with $y_{N+1} = \frac{1}{2}(z_1 + z_2)$

## -N**3*Energy of Hydrogen Atom
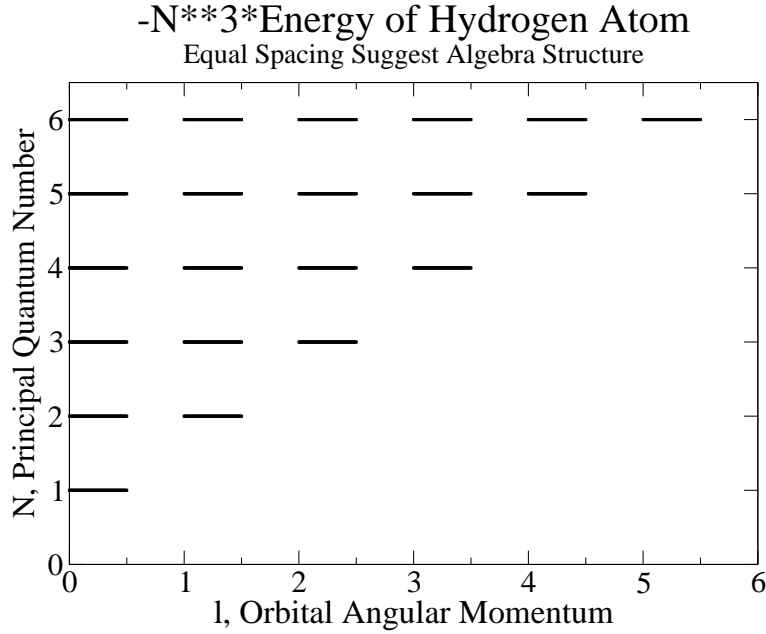### Equal Spacing Suggest Algebra Structure



Fig. 14.2. Nonrelativistic spectrum of the hydrogen atom, replotted to emphasize the possibility of a dynamical algebra.

and $y_{N+2} = \frac{1}{2}(z_1 - z_2)$:

$$
\left[ \begin{array}{c|cc} G & & \\ \hline & & -\frac{1}{2} \\ & -\frac{1}{2} & \end{array} \right] \begin{array}{c} \mathbf{y} \\ \\ z_1 \\ z_2 \end{array}
\qquad
\left[ \begin{array}{c|cc} G & & \\ \hline & -1 & \\ & & +1 \end{array} \right] \begin{array}{c} \mathbf{y} \\ \\ y_{N+1} \\ y_{N+2} \end{array}
$$

$$\tag{14.38}$$

The conformal conditon Eq.(14.37) defines a cone in the enlarged $N+2$ dimensional space. If the group that preserves the metric $G$ in $R^N$ is $SO(p,q)$ the group that preserves the metric in $R^{N+2}$ is $SO(p+1, q+1)$. We seek to construct a spherical or hyperbolic slice of this cone.

The connection with the Kepler problem is made as follows. The momenta $\mathbf{p}$ are lifted to the coordinates on a sphere $S^3 \subset R^4$ ($E < 0$) or a two-sheeted hyperboloid $H^3 \subset R^4$ ($E > 0$) by the following projective

transformations:

$$\hat{\mathbf{u}} = \frac{\frac{1}{2}(p_0^2 - \mathbf{p} \cdot \mathbf{p})}{\frac{1}{2}(p_0^2 + \mathbf{p} \cdot \mathbf{p})} \, \mathbf{w} + \frac{p_0 \mathbf{p}}{\frac{1}{2}(p_0^2 + \mathbf{p} \cdot \mathbf{p})} \qquad E < 0$$

$$\hat{\mathbf{u}} = \frac{\frac{1}{2}(p_0^2 + \mathbf{p} \cdot \mathbf{p})}{\frac{1}{2}(p_0^2 - \mathbf{p} \cdot \mathbf{p})} \, \mathbf{w} + \frac{p_0 \mathbf{p}}{\frac{1}{2}(p_0^2 - \mathbf{p} \cdot \mathbf{p})} \qquad E > 0$$

$$(14.39)$$

For the 4-vectors $\mathbf{u}$ the metric $G$ that appears in Eq.(14.38) is determined from the denominators in Eq.(14.39):

$$\mathbf{u}^t G \mathbf{u} = u_0^2 \pm \sum_{i=1}^{3} u_i^2 \qquad \begin{array}{ll} + & \text{for} \quad E < 0 \\ - & \text{for} \quad E > 0 \end{array} \qquad (14.40)$$

The algebraic surfaces on which the projective vector $\mathbf{u}$ lies is defined by the condition $\mathbf{u}^t G \mathbf{u} = 1$.

The connection with the conformal transformations introduced above is as follows. The group that leaves invariant the conformal metric diag $(1, \pm I_3, -1, +1)$ is $SO(5,1)$ for $E < 0$ and $SO(2,4)$ for $E > 0$. On the surfaces (sphere, hyperboloid) the condition $\mathbf{u}^t G \mathbf{u} = 1$ is satisfied, so that $z_1 = z_2$, $y_4 = \lambda$ and $y_5 = 0$ (the six coordinates are labeled $(y_0, \mathbf{y} = \lambda \mathbf{u}, y_4 = \frac{1}{2}(z_1 + z_2), y_5 = \frac{1}{2}(z_1 - z_2))$. Transformations that map the algebraic surface to itself must map $y_5 = 0$ to $y_5 = 0$. It is a simple matter to verify that this is the matrix subgroup of the $6 \times 6$ matrix group $SO(5,1)$ or $SO(2,4)$ of the form $\begin{bmatrix} M & 0 \\ 0 & 1 \end{bmatrix}$, with $M$ a $5 \times 5$ matrix that preserves the metric diag $(1, \pm I_3, -1)$ in $R^5$. This is $SO(4,1)$ for $E < 0$ and $SO(1,4)$ for $E > 0$.

It remains to show that this group maps these algebraic surfaces into themselves. To this end we write the linear transformation in $R^5$ as follows

$$\begin{bmatrix} \lambda \mathbf{u} \\ \lambda \end{bmatrix}' = \begin{bmatrix} A & B \\ C & D \end{bmatrix} \begin{bmatrix} \lambda \mathbf{u} \\ \lambda \end{bmatrix} \qquad (14.41)$$

where $A$ is a $4 \times 4$ matrix, etc. From this we determine

$$\mathbf{u}' = \frac{A(\lambda \mathbf{u}) + B\lambda}{C(\lambda \mathbf{u}) + D\lambda} \qquad (14.42)$$

The inner product of $\mathbf{u}'$ with itself satisfies

$$(\mathbf{u}')^t G \mathbf{u}' - 1 = \frac{(A\lambda \mathbf{u} + B\lambda)^t G(A\lambda \mathbf{u} + B\lambda) - (C\lambda \mathbf{u} + D\lambda)^t (C\lambda \mathbf{u} + D\lambda)}{(C\lambda \mathbf{u} + D\lambda)^t (C\lambda \mathbf{u} + D\lambda)}$$

$$(14.43)$$

By using the relations among the submatrices required by the metric preserving condition (e.g., $A^t G A - C^t C = G$, etc.) it is a simple matter to show that this reduces to

$$(\mathbf{u}', \mathbf{u}')_N - 1 = \frac{(\mathbf{u}, \mathbf{u})_N - 1}{(C\mathbf{u} + D)^t (C\mathbf{u} + D)} \tag{14.44}$$

In short, the algebraic surface is invariant under this transformation group.

**Remark:** The subgroup $SO(4)$ rigidly rotates the sphere $S^3 \subset R^4$ into itself while the subgroup $SO(3,1)$ "rigidly rotates" the hyperboloid into itself. In the latter case this is less intuitive. This means that the coordinates of the hyperboloid are mapped into themselves by a *linear* transformation in $R^4$. The group $SO(4,1)$ maps coordinates in these spaces to themselves through a *nonlinear* transformation in $R^4$: in this case a simple projective transformation. It is a linear transformation in $R^5$.

The infinitesimal generators of this nonlinear transformation are constructed as follows [3, 4]. For $E < 0$ introduce a 4-vector $u$ as usual $(u_0 \rightarrow u_4)$

$$\begin{aligned}
\mathbf{u} &= 2p_4(\mathbf{p} \cdot \mathbf{p} + p_4^2)^{-1}\mathbf{p} \\
u_4 &= (\mathbf{p} \cdot \mathbf{p} - p_4^2)(\mathbf{p} \cdot \mathbf{p} + p_4^2)^{-1}
\end{aligned} \tag{14.45}$$

Define the 4-vector B in terms of the 4-vector $u$ and the angular momentum vector $\mathbf{L}$ and the scaled (by $1/\sqrt{2m|E|}$) Runge-Lenz vector $\mathbf{M}'$ as follows:

$$\begin{aligned}
\mathbf{B} &= \mathbf{M}'u_4 + \mathbf{L} \times \mathbf{u} - \tfrac{3}{2}i\mathbf{u} &= \tfrac{i}{2}\left[\mathbf{u}, \mathbf{L}^2 + \mathbf{M}'^2\right] \\
B_4 &= \mathbf{M}' \cdot \mathbf{u} + \tfrac{3}{2}i\mathbf{u} &= \tfrac{i}{2}\left[u_4, \mathbf{L}^2 + \mathbf{M}'^2\right]
\end{aligned}$$

The operators $L_i$, $M_i'$, and $B_\mu$ are the infinitesimal generators of $SO(4,1)$ as follows, for $E < 0$.

$$\left[\begin{array}{cccc|c}
0 & L_3 & -L_2 & M_1 & B_1 \\
-L_3 & 0 & L_1 & M_2 & B_2 \\
L_2 & -L_1 & 0 & M_3 & B_3 \\
-M_1 & -M_2 & -M_3 & 0 & B_4 \\
\hline
B_1 & B_2 & B_3 & B_4 & 0
\end{array}\right] \begin{array}{c} + \\ + \\ + \\ + \\ - \end{array}$$

### 14.9    Conformal Symmetry $SO(4,2)$

The largest set of transformations that leave the states of the hydrogen atom invariant, in some sense, is the conformal group $SO(4,2)$. Several different ways have been developed to prove this point. We review three here.

### *14.9.1    Schwinger Representation*

The algebra of the dynamical symmetry group has infinitesimal generators $\mathbf{L}$ and $\mathbf{M'}$. Their linear combinations given two sets of vector operators $\mathbf{A}$ and $\mathbf{B}$ that mutually commute and have angular momentum commutation relations on bound states. It is possible to represent these operators using the boson representation. That is, for the operators $\mathbf{A}$ we introduce annihilation and creation operators $a_i, a_j^\dagger$ for two independent modes, and similarly we introduce operators $b_i, b_j^\dagger$ to describe $\mathbf{B}$. Basis states on which these operators act have the form $|m_1, m_2; n_1, n_2\rangle$ where, for example

$$a_1^\dagger a_2 |m_1, m_2; n_1, n_2\rangle \quad = \quad |m_1 + 1, m_2 - 1; n_1 n_2\rangle \sqrt{m_1 + 1}\sqrt{m_2}$$

$$b_1^\dagger b_1 |m_1, m_2; n_1, n_2\rangle \quad = \quad |m_1, m_2; n_1 n_2\rangle (\sqrt{n_1})^2$$

The orthogonality of $\mathbf{L}$ and $\mathbf{M}$ leads to the orthogonality of $\mathbf{A}$ and $\mathbf{B}$, and this leads directly to the condition $j_a = j_b$, where $j_a = \frac{1}{2}(m_1 + m_2)$ and $j_b = \frac{1}{2}(n_1 + n_2)$.

From the previous section we know there is a group that maps bound states into (linear combinations of) bound states. We determine an algebra of operators that performs the same function on bound states as follows. Operators that change the principle quantum number $N = 2j_a + 1 = 2j_b + 1 = (j_a + j_b) + 1$ must change $j_a = j_b$. Operators that change $j_a$ have the form $a_i^\dagger$ or $a_i^\dagger a_j^\dagger$, but they do not simultaneously change $j_b$. Only operators that simultaneously add or subtract one excitation to the subsystems $A$ and $B$ simultaneously maintain the constraint $j_a = j_b$. The largest set of operators bilinear in the boson operators that map hydrogen atom bound states to bound states consists of the operators

| Operators | $a_i^\dagger a_j$ | $b_i^\dagger b_j$ | $a_i^\dagger b_j^\dagger$ | $a_i b_j$ | |
|---|---|---|---|---|---|
| Subalgebra | $\mathfrak{u}(2)$ | $\mathfrak{u}(2)$ | | | (14.46) |
| Number | 4 | 4 | 4 | 4 | |

What is this algebra? Among these 16 operators, the maximal number

of mutually commuting operators that can be found is four. These are conveniently chosen as the number operators for the four boson modes: $(H_1, H_2, H_3, H_4) = (a_1^\dagger a_1, a_2^\dagger a_2, b_1^\dagger b_1, b_2^\dagger b_2)$. The remaining twelve operators have eigenoperator commutation relations with this set:

$$
\begin{array}{llll}
a_1^\dagger a_2 & (+1,-1,0,0) & a_1^\dagger b_1^\dagger & (+1,0,+1,0) & a_1 b_1 & (-1,0,-1,0) \\
a_2^\dagger a_1 & (-1,+1,0,0) & a_1^\dagger b_2^\dagger & (+1,0,0,+1) & a_1 b_2 & (-1,0,0,-1) \\
b_1^\dagger b_2 & (0,0+1,-1) & a_2^\dagger b_1^\dagger & (0,+1,+1,0) & a_2 b_1 & (0,-1,-1,0) \\
b_2^\dagger b_1 & (0,0,-1,+1) & a_2^\dagger b_2^\dagger & (0,+1,0,+1) & a_2 b_2 & (0,-1,0,-1)
\end{array}
$$

$$\tag{14.47}$$

All these roots have equal length, and inner products among these roots are all $\pm\frac{1}{2}$ or 0. The operator

$$(a_1^\dagger a_1 + a_2^\dagger a_2) - (b_1^\dagger b_1 + b_2^\dagger b_2)$$

commutes with all operators in this set. It is a constant of motion, and in fact vanishes on all hydrogen atom bound states. As a result the algebra is the direct sum of an abelian invariant subalgebra spanned by this operator, and a rank-three simple Lie algebra, all of whose roots have equal lengths and are either orthogonal or make angles of $\frac{\pi}{4}$ or $\frac{3\pi}{4}$ radians with each other. The algebra is uniquely a real form of $A_3 = D_3$.

Which real form? It is possible to form a number of subalgebras of type $A_1$ from these operators:

$$
\begin{array}{llll}
a_1^\dagger a_2 & a_2^\dagger a_1 & \frac{1}{2}(a_1^\dagger a_1 - a_2^\dagger a_2) & \mathfrak{su}(2) \\
b_1^\dagger b_2 & b_2^\dagger b_1 & \frac{1}{2}(b_1^\dagger b_1 - b_2^\dagger b_2) & \mathfrak{su}(2) \\
a_i^\dagger b_j^\dagger & a_i b_j & \frac{1}{2}(a_i^\dagger a_i + b_j^\dagger b_j + 1) & \mathfrak{su}(1,1)
\end{array}
$$

The first two are compact, the last four are not compact. The maximal compact subalgebra is spanned by the two compact subalgebras together with the diagonal operator $a_1^\dagger a_1 + a_2^\dagger a_2 + b_1^\dagger b_1 + b_2^\dagger b_2$. This is the algebra $\mathfrak{so}(4)+\mathfrak{so}(2)$. The fifteen dimensional Lie algebra that maps bound states to bound states is therefore $\mathfrak{so}(4,2) = \mathfrak{su}(2,2)$. This is the conformal algebra.

### 14.9.2    Dynamical Mappings

Although the classical Kepler problem is analytically solvable, analyticity disappears under perturbation. In this case classical orbits must be computed numerically. At points of very close approach the velocity of the particles increases greatly, so it is prudent to slow down the

integration time step to preserve accuracy. This procedure has been im-
plemented formally through a canonical transformation [48, 67], and is
now widely known as the Kustaanheimo-Stiefel transformation. Under
this transformation time is stretched out when the distance $R$ between
the interacting particles becomes small. In addition the (relative) co-
ordinates are projected from $R^3$ to a fictitious space $R^4$. Under this
transformation, and a constraint, the Kepler hamiltonian is transformed
into a four dimensional harmonic oscillator hamiltonian.

Coordinates $(q_1, q_2, q_3, q_4)$ in the fictitions space $R^4$ are related to
coordinates $(Q_1, Q_2, Q_3)$ in the real space by the $4 \times 4$ transformation

$$
\begin{bmatrix} Q_1 \\ Q_2 \\ Q_3 \\ Q_4 \end{bmatrix} = M_{KS} \begin{bmatrix} q_1 \\ q_2 \\ q_3 \\ q_4 \end{bmatrix} = \begin{bmatrix} q_1 & -q_2 & -q_3 & q_4 \\ q_2 & q_1 & -q_4 & -q_3 \\ q_3 & q_4 & q_1 & q_2 \\ q_4 & -q_3 & q_2 & -q_1 \end{bmatrix} \begin{bmatrix} q_1 \\ q_2 \\ q_3 \\ q_4 \end{bmatrix} \tag{14.48}
$$

The transformation is constructed so that the "fourth" real coordinate
$Q_4$ is identically zero. This transformation is invertible provided $q_1^2 +
q_2^2 + q_3^2 + q_4^2 \neq 0$. The distance $R = \sqrt{Q_1^2 + Q_2^2 + Q_3^2}$ in $R^3$ and the
distance $q = \sqrt{q_1^2 + q_2^2 + q_3^2 + q_4^2}$ in $R^4$ are related by: $R = q^2$.

The other half of the canonical transformation, involving the momenta
in the real and fictitious spaces, is

$$
(P_1, P_2, P_3, P_4)^t = \frac{1}{2R} M_{KS}(p_1, p_2, p_3, p_4)^t
$$

A constraint condition must be applied to force $P_4 = 0$. This condition
is

$$
\zeta = -2RP_4 = (q_1 p_4 - q_4 p_1) + (q_3 p_2 - q_2 p_3) = 0 \tag{14.49}
$$

With this constraint we find $P^2 = P_1^2 + P_2^2 + P_3^2 = \frac{1}{4R} p^2 - \frac{\zeta^2}{4R^2} \rightarrow \frac{1}{4R}(p_1^2 + p_2^2 + p_3^2 + p_4^2)$. With these transformations the hamiltonian in
the real space can be transformed to a hamiltonian in the fictitious space
by

$$
\frac{P^2}{2m} - \frac{e^2}{R} = E \xrightarrow{\times R} \frac{R\,P^2}{2m} - e^2 = E\,R \xrightarrow{KS} \frac{p^2}{8m} - e^2 = E\,q^2 \tag{14.50}
$$

This is the hamiltonian for a four-dimensional harmonic oscillator when
$E < 0$, as easily seen by rearranging the terms

$$
\frac{p^2}{2m} - 4Eq^2 = 4e^2 \tag{14.51}
$$

The angular momentum operators in the real and fictitious spaces are bilinear products of the position and momentum coordinates, as follows:

$$(Q_1, Q_2, Q_3, Q_4) \begin{bmatrix} 0 & \theta_3 & -\theta_2 & * \\ -\theta_3 & 0 & \theta_1 & * \\ \theta_2 & -\theta_1 & 0 & * \\ -* & -* & -* & 0 \end{bmatrix} \begin{bmatrix} P_1 \\ P_2 \\ P_3 \\ P_4 \end{bmatrix}$$

$$\frac{1}{2}(q_1, q_2, q_3, q_4) \begin{bmatrix} 0 & \theta_3 & -\theta_2 & \theta_1 \\ -\theta_3 & 0 & \theta_1 & \theta_2 \\ \theta_2 & -\theta_1 & 0 & \theta_3 \\ -\theta_1 & -\theta_2 & -\theta_3 & 0 \end{bmatrix} \begin{bmatrix} p_1 \\ p_2 \\ p_3 \\ p_4 \end{bmatrix} \qquad (14.52)$$

Similar expressions can be given for the Runge-Lenz vector. However, these are quadratic in the position and momentum operators. As a result they must be expressed in matrix form using $8 \times 8$ matrices acting on the vector $(q_1, q_2, q_3, q_4; p_1, p_2, p_3, p_4)$ on the left and its transpose on the right [59].

We now ask: what is the largest group of transformations on the coordinates and momenta that:

**a.** is linear
**b.** is canonical
**c.** preserves $\zeta = 0$.

We address this question in the usual way. Linear transformations allow us to use matrices. These are $8 \times 8$ matrices acting on the four coordinates and four momenta. Preserving the Poisson brackets requires that the matrices satisfy a symplectic metric-preserving condition: $M^t G_1 M = G_1$. Preserving the condition $\zeta = 0$ requires these transformations to satisfy another metric-preserving condition: $M^t G_2 M = G_2$.

The matrices $G_i$ have the form $G_i = \begin{bmatrix} 0 & M_i \\ -M_i & 0 \end{bmatrix}$, where

$$M_1 = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \qquad M_2 = \begin{bmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & -1 & 0 \\ 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{bmatrix}$$

$$M_1^t = +M_1 \quad G_1^t = -G_1 \qquad\qquad M_2^t = -M_2 \quad G_2^t = +G_2$$
$$(14.53)$$

The metric $G_1$ is antisymmetric and the metric $G_2$ is symmetric, with

signature $(+4, -4)$. The group that preserves the antisymmetric metric is $Sp(8; R)$ and the group that preserves the symmetric metric is $SO(4, 4)$. The group that satisfies both metric-preserving conditions is their intersection:

$$Sp(8; R) \cap SO(4, 4) = SU(2, 2) \simeq SO(4, 2) \qquad (14.54)$$

The simplest way to see this result is to perform a canonical transformations from coordinates $(q, p)$ to coordinates $(s, r)$:

$$\begin{bmatrix} s_1 \\ r_4 \end{bmatrix} = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ -1 & 1 \end{bmatrix} \begin{bmatrix} q_1 \\ p_4 \end{bmatrix} \qquad \begin{bmatrix} s_2 \\ r_3 \end{bmatrix} = \frac{1}{\sqrt{2}} \begin{bmatrix} -1 & 1 \\ -1 & -1 \end{bmatrix} \begin{bmatrix} q_2 \\ p_3 \end{bmatrix}$$

$$\begin{bmatrix} s_3 \\ r_2 \end{bmatrix} = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ -1 & 1 \end{bmatrix} \begin{bmatrix} q_3 \\ p_2 \end{bmatrix} \qquad \begin{bmatrix} s_4 \\ r_1 \end{bmatrix} = \frac{1}{\sqrt{2}} \begin{bmatrix} -1 & 1 \\ -1 & -1 \end{bmatrix} \begin{bmatrix} q_4 \\ p_1 \end{bmatrix}$$
$$(14.55)$$

Since the new coordinates are already canonical, only the condition $\zeta = 0$ remains to be satisfied. It is a simple matter to verify that

$$z_1 = \frac{1}{\sqrt{2}}(s_1 + is_2) \quad z_2 = \frac{1}{\sqrt{2}}(r_1 + ir_2)$$

$$z_3 = \frac{1}{\sqrt{2}}(s_3 + is_4) \quad z_4 = \frac{1}{\sqrt{2}}(r_3 + ir_4)$$

$$z_1^* z_1 - z_2^* z_2 + z_3^* z_3 - z_4^* z_4 = \zeta$$

$$(14.56)$$

The noncompact group $U(2, 2)$ preserves the constraint Eq.(14.49).

### 14.9.3    Lie Algebra of Physical Operators

A number of workers have shown that the Hamiltonian describing the interaction of a charged particle interacting with an external Coulomb field $[V(r) = -e^2/r]$ can be expressed in terms of operators that close under commutation. The Lie algebra that these operators span is isomorphic with the Lie algebra of a noncompact orthogonal group.

Three vector operators and a scalar operator

$$\begin{array}{lll} \mathbf{J} &=& \mathbf{r} \times \mathbf{p} & \text{Angular Momentum} \\ \mathbf{M} &=& \frac{1}{2m}\mathbf{p} \times \mathbf{L} - \mathbf{L} \times \mathbf{p} - K\frac{\mathbf{r}}{r} & \text{Laplace Runge Lenz vector} \\ \mathbf{A} &=& \frac{1}{2m}\mathbf{p} \times \mathbf{L} - \mathbf{L} \times \mathbf{p} + K\frac{\mathbf{r}}{r} & \text{Dual vector} \\ A_4 &=& \mathbf{r} \cdot \mathbf{p} + \frac{3}{2}\frac{\hbar}{i} & \text{Dual scalar} \end{array}$$

$$(14.57)$$

close under commutation to span a Lie algebra that is isomorphic with $\mathfrak{so}(4, 1)$.

Five additional operators can be introduced that extend the algebra to $\mathfrak{so}(4,2)$. These include one vector operator and two additional operators:

$$
\begin{aligned}
\Gamma_i &= r\mathbf{p}_i \\
\Gamma_4 &= \tfrac{1}{2}(r\mathbf{p}\cdot\mathbf{p} - r) \\
\Gamma_5 &= \tfrac{1}{2}(r\mathbf{p}\cdot\mathbf{p} + r)
\end{aligned}
\tag{14.58}
$$

The commutation relations that these 15 operators satisfy are summarized by the $6 \times 6$ matrix

$$
\left[
\begin{array}{cccc|cc}
0 & J_3 & -J_2 & M_1 & A_1 & \Gamma_1 \\
-J_3 & 0 & J_1 & M_2 & A_2 & \Gamma_2 \\
J_2 & -J_1 & 0 & M_3 & A_3 & \Gamma_3 \\
-M_1 & -M_2 & -M_3 & 0 & A_4 & \Gamma_4 \\ \hline
A_1 & A_2 & A_3 & A_4 & 0 & \Gamma_5 \\
\Gamma_1 & \Gamma_2 & \Gamma_3 & \Gamma_4 & -\Gamma_5 & 0
\end{array}
\right]
\begin{array}{c}
+ \\ + \\ + \\ + \\ - \\ -
\end{array}
$$

The four triplets $J_i, M_i, A_i, \Gamma_i$ $(i = 1,2,3)$ have transformation properties of three-vectors under rotations. The three additional operators $A_4, \Gamma_4, \Gamma_5$ close under commutation and span a Lie algebra that is isomorphic with $\mathfrak{so}(2,1)$.

The Schrödinger and Klein-Gordon Hamiltonians for an electron of charge $-e$ in the Coulomb field $\Phi(r) = e/r$ of a proton can be expressed in terms of operators of type $A_4, \Gamma_4$, and $\Gamma_5$. These operators are displayed in Table 14.3, along with the Hamiltonians and the algebraic representation of the wave equations.

## 14.10    Spin Angular Momentum

The interaction of the electron with the electromagnetic field is properly described by the Dirac equation. The electromagnetic field $(\mathbf{E}, \mathbf{B})$ is described by the four-vector potential $A_\mu = (\phi, \mathbf{A})$. The electron has charge $q = -e$ (where $e$ is the charge on the proton) and spin $\frac{1}{2}$. The Dirac equation $H_D\psi = E\psi$ is a matrix differential equation of first order:

$$
H_D = -e\phi(r) + \beta mc^2 + \gamma \cdot (c\mathbf{p} + e\mathbf{A})
\tag{14.59}
$$

The $4 \times 4$ matrices $\beta$ and $\gamma_i$ can be chosen as

$$
\beta = \left[\begin{array}{cc} I_2 & 0 \\ 0 & -I_2 \end{array}\right]
\qquad
\gamma_i = \left[\begin{array}{cc} 0 & \sigma_i \\ \sigma_i & 0 \end{array}\right]
\tag{14.60}
$$

Table 14.3. *Nonrelativistic and relativistic Hamiltonians for a spinless particle, operator representation of the operators $A_4, \Gamma_4$, and $\Gamma_5$, expression of the Hamiltonians and wave equations in terms of these operators, and explicit values of the coefficients in these equations. In the event a magnetic field $\mathbf{B}$ is present, the momentum operators $\mathbf{p}$ should be replaced by $\pi = \mathbf{p} - \frac{q}{c}\mathbf{A}$. Under this condition the operators still close under commutation.*

| | | |
|---|---|---|
| $H$ | $\dfrac{p^2}{2m} - \dfrac{\alpha}{r}$ | $\sqrt{p^2 + m^2} - \frac{\alpha}{r}$ |
| $A_4$ | $\mathbf{r}\cdot\mathbf{p} - i$ | $\mathbf{r}\cdot\mathbf{p} - i$ |
| $\Gamma_4$ | $\frac{1}{2}(r\mathbf{p}\cdot\mathbf{p} - r)$ | $\dfrac{1}{2}(r\mathbf{p}\cdot\mathbf{p} - r - \dfrac{\alpha^2}{r})$ |
| $\Gamma_5$ | $\frac{1}{2}(r\mathbf{p}\cdot\mathbf{p} + r)$ | $\dfrac{1}{2}(r\mathbf{p}\cdot\mathbf{p} + r - \dfrac{\alpha^2}{r})$ |
| $\Theta$ | $r(H_S - W)$ | $r\left\{\left(H_{KG} + \dfrac{\alpha}{r}\right)^2 - \left(E + \dfrac{\alpha}{r}\right)^2\right\}$ |
| | $A(\Gamma_5 + \Gamma_4) + B(\Gamma_5 - \Gamma_4) + C$ | $A(\Gamma_5 + \Gamma_4) + B(\Gamma_5 - \Gamma_4) + C$ |
| $A$ | $1/2m$ | $1$ |
| $B$ | $-W$ | $m^2 - E^2$ |
| $C$ | $-\alpha$ | $-2\alpha E$ |

Here $\sigma_i$ are the standard Pauli $2 \times 2$ spin matrices (cf., Eq. (3.39), Problem 3.1).

The 15 dimensional Lie algebra for the Dirac equation is spanned by the operators $\mathbf{J}, \mathbf{M}, \mathbf{A}, \mathbf{\Gamma}$ as given in Eq. (14.57), and the three operators $A_4, \Gamma_4, \Gamma_5$. The latter two are modified to allow a treatment of the Dirac operator along the same lines as the treatment of the Schrödinger and Klein-Gordon operators given in Subsection 14.9.3. We define operators

$$
\begin{aligned}
M_4 &= \mathbf{r}\cdot\mathbf{p} - i \\
\Gamma_4 &= \frac{1}{2}\left\{(r\mathbf{p}\cdot\mathbf{p} - r - \frac{\alpha^2}{r} - \frac{i\alpha\gamma\cdot\mathbf{r}}{r^2})\right\} \\
\Gamma_5 &= \frac{1}{2}\left\{(r\mathbf{p}\cdot\mathbf{p} + r - \frac{\alpha^2}{r} - \frac{i\alpha\gamma\cdot\mathbf{r}}{r^2}\right\}
\end{aligned}
\tag{14.61}
$$

As before, the substitution $\mathbf{p} \to \pi = \mathbf{p} - \frac{q}{c}\mathbf{A}$ is in order in the event there is a nonzero magnetic field $\mathbf{B}$. These operators close under commutation to form an $\mathfrak{so}(2,1)$ Lie algebra. These operators also close under commutation with the four three-vectors $J_i, M_i, A_i, \Gamma_i$ defined in Table 14.3. The Dirac hamiltonian is expressed in terms of these generators as follows:

$$\Theta \;=\; r\left\{\left(H_D + \frac{\alpha}{r}\right)^2 - \left(E + \frac{\alpha}{r}\right)^2\right\}$$

$$\;=\; A(\Gamma_5 + \Gamma_4) + B(\Gamma_5 - \Gamma_4) + C \tag{14.62}$$

where the coefficients $A, B, C$ have exactly the same values as for the Klein-Gordon operator (cf., Table 14.3). In short, the operators $\Gamma_4, \Gamma_5$ are modified but the relation among these operators in the algebraic representation of the relativistic wave equations is not.

## 14.11    Spectrum Generating Group

The physics of the hydrogenic problem is determined primarily by the radial equation Eq. (14.9). It is possible to determine solutions of this equation using operators that close under commutation. These are the generators of a Lie algebra. The corresponding group is called a spectrum generating group.

To construct a set of operators that close under commutation, we first simplify the radial equation by multiplying on the left by $r$

$$\left(rD^2 + \frac{A}{r} + B + Cr\right) R(r) = 0 \tag{14.63}$$

with $D = d/dr$. The operators $r$ and $D$ behave under commutation like the boson creation and annihilation operators $a^\dagger$ and $a$. In fact, the nonzero commutation relations are

$$[rD, r] \;=\; +r \qquad\qquad \left[a^\dagger a, a^\dagger\right] \;=\; +a^\dagger$$

$$\left[rD, rD^2\right] \;=\; -rD^2 \qquad \left[a^\dagger a, a^\dagger a a\right] \;=\; -a^\dagger a a \tag{14.64}$$

$$\left[r, rD^2\right] \;=\; -2rD \qquad \left[a^\dagger, a^\dagger a a\right] \;=\; -2a^\dagger a$$

The linear combinations $rD^2 + r$ and $rD^2 - r$ are compact and non-compact, respectively. In order to model the differential operator Eq. (14.63) with a set of operators that close under commutation to form a finite-dimensional Lie algebra, we must be careful, as

$$\left[rD, \frac{1}{r}\right] = -\frac{1}{r}$$

$$\left[rD^2, \frac{1}{r}\right] = \frac{2}{r^2} - \frac{1}{r}D$$

We choose as operators in the Lie algebra $\mathfrak{so}(2,1)$ the three differential operators

$$\Gamma_5 = \frac{1}{2}\left(rD^2 + \frac{a}{r} - r\right)$$

$$\Gamma_4 = \frac{1}{2}\left(rD^2 + \frac{a}{r} + r\right) \qquad (14.65)$$

$$M_4 = rD$$

The Casimir operator for this algebra is $C^2 = \Gamma_5^2 - \Gamma_4^2 - M_4^2 = -a$. The representations of this algebra have been described in Problem 11.6.

The radial equation Eq. (14.63) is expressed in terms of the three operators as follows $(a \rightarrow A)$

$$((\Gamma_5 + \Gamma_4) + B + C(\Gamma_4 - \Gamma_5)) R(r) = 0 \qquad (14.66)$$

Next, we rotate the generators of the algebra according to

$$e^{\theta M_4}\begin{pmatrix}\Gamma_5 \\ \Gamma_4\end{pmatrix}e^{-\theta M_4} = \begin{bmatrix}\cosh\theta & -\sinh\theta \\ -\sinh\theta & \cosh\theta\end{bmatrix}\begin{pmatrix}\Gamma_5 \\ \Gamma_4\end{pmatrix} \qquad (14.67)$$

When this similarity transformation is applied to Eq.(14.66) we obtain the following result:

$$\left[\left(e^{-\theta} - C\,e^{\theta}\right)\Gamma_5 + \left(e^{-\theta} + C\,e^{\theta}\right)\Gamma_4 + B\right]e^{\theta M_4}R(r) = 0 \qquad (14.68)$$

The rotation angle $\theta$ can be chosen to eliminate either the noncompact generator $\Gamma_4$ or the compact generator $\Gamma_5$, depending on the sign of the parameter $C$.

### 14.11.1     Bound States

If $C < 0$ we can choose $e^{-\theta} + C\,e^{\theta} = 0$, so that the resulting equation becomes

$$\left(2\sqrt{-C}\,\Gamma_5 + B\right)u(r) = 0 \tag{14.69}$$

where $u(r) = e^{\theta M_4}R(r)$. If $A$ is the Casimir invariant of this representation of $\mathfrak{su}(1,1)$, the discrete spectrum of the compact operator $\Gamma_5$ is $N = -\frac{1}{2} + \sqrt{(\frac{1}{2})^2 - A} + 1 + n$, $n = 0, 1, 2, \ldots$ . This result leads directly to the eigenvalue spectrum for the nonrelativistic and the relativistic hydrogen atom (no spin) obtained in Eq. (14.12).

**Remark:** The spectrum generating algebra Eq. (14.65) acts in Hilbert spaces that carry unitary irreducible representations of the noncompact group $SO(2,1)$. These representations are indexed by an integer $l$ that has an interpretation as angular momentum. The energy spectrum that we have computed has the behavior (in the nonrelativistic case) $W = -\frac{1}{2}mc^2\alpha^2\frac{1}{(N)^2}$, where $N = l + 1 + k$, $k = 0, 1, 2, \ldots$. Here $N$ is the principle quantum number. The result is that this algebra acts to change the principle quantum number while keeping $l$ constant. Since the three operators in the spectrum generating algebra commute with the angular momentum operators, the quantum number $m_l$ (eigenvalue of $L_z$) is also invariant under the action of these operators. The states connected by the operators of this $\mathfrak{so}(2,1)$ algebra are $|N, lm\rangle \leftrightarrow |N \pm 1, lm\rangle$. The states on which these operators act are organized in "angular momentum towers." These states are organized vertically in Fig 14.2.

**Remark:** The angular momentum operators $L_z, L_\pm$ act on multiplets shown as a single horizontal line in Figs. 14.1 and 14.2. The operators $M_z, M_\pm$ associated with the Laplace-Runge-Lenz vector act horizontally on the levels shown in these two figures. The operators $\Gamma_z, \Gamma_\pm = \Gamma_4 \pm iM_4$ act vertically on the levels shown in these figures. Since $[\mathbf{L}, \Gamma] = 0$, the operators $\Gamma$ do not change the $m$ values of hydrogenic states.

**Remark:** The shift down operator $\Gamma_-$ annihilates the ground state in a given angular momentum tower: $\Gamma_-\langle r|N \begin{smallmatrix} l = N - 1 \\ m \end{smallmatrix} \rangle = 0$. Since the differential operators are known, this relation can be used, as was the relation $L_-Y^l_{m=-l}(\theta, \phi) = 0$, to determine the radial wavefunction $\langle r|N, l = N - 1\rangle$.

### *14.11.2    Scattering States*

If $C > 0$ we can choose $\theta$ so that $e^{-\theta} - C\,e^{\theta} = 0$. Eq. (14.66) reduces to

$$\left(2\sqrt{C}\,\Gamma_4 + B\right)u(r) = 0 \qquad\qquad (14.70)$$

where as before $u(r) = e^{\theta M_4}R(r)$. Since the generator $\Gamma_4$ is noncompact, it has a continuous spectrum. The energy can be written in terms of the scaling factor $k \simeq e^{-\theta}$ with $E = \hbar^2 k^2/2m$. The asymptotic form of the wave function is [38, 47]

$$R_{k,l}(r) \sim \sqrt{\frac{2}{\pi}}\sin\left(kr - \frac{\pi}{2}\,j + \frac{\alpha}{k}(\log(2kr) + \delta(j))\right) \qquad (14.71)$$

where $\delta(j) = \arg\left[\Gamma(j+1-i(\alpha/k)\right]$ is part of the scattering phase shift, and the expression for $j$ is given by $j = -\frac{1}{2} + \sqrt{(\frac{1}{2})^2 - A}$.

### 14.11.3     Quantum Defect

Multielecton atoms are complicated objects. If one of the electrons is promoted to a high lying level, it is on average far from the nucleus and the core electrons. Some simplifications can then be made in the description of its excited state spectrum. As the "Rydberg" electron approaches the core, the positive nuclear charge is less completely screened by the core electrons, and the electron is more strongly attracted than a simple $-1/r$ potential suggests. It is possible to represented this extra attraction by adding a term of the form $-1/r^2$ to the potential to represent penetration of the core electrons. To this end the potential used in the Schrödinger and Klein-Gordon equations is $V(r) = -\frac{e^2}{r} \rightarrow -e^2/r - \mu_l(\hbar^2/2m)/r^2$. This perturbation produces a modification in the radial equation. The modification is encapsulated entirely in the change

$$A \rightarrow A' = A + \mu_l \qquad\qquad (14.72)$$

This change produces a change in the value of $j \rightarrow j' = j + \Delta j$, where $\Delta j = -\mu_l/(2l+1)$ in the nonrelativistic case. This change produces a change in the bound state energy spectrum:

$$E_{N=n+l+1} = -\frac{mc^2\alpha^2}{2N^2} \rightarrow -\frac{mc^2\alpha^2}{2(N+\Delta j)^2} \qquad (14.73)$$

The quantum defect $\Delta j$ causes the Rydberg states to be bound more strongly than in a pure hydrogenic atom (without screening). The same

change occurs in scattering states. There is an additional phase shift due to the stronger attraction in the core. The excess phase shift is

$$\Delta\phi = -\frac{\pi}{2}\,\Delta j + \frac{\alpha}{\pi}\,\arg\left(\Gamma[j+1+\Delta j - i(\alpha/k)] - \Gamma[j+1-i(\alpha/k)]\right)$$
$$(14.74)$$

**Remark:** More accurate calculations of bound state spectra and scattering phase shifts employ more accurate representations of core screening (than $-1/r^2$). Nevertheless, the results are the same: A quantum defect in the bound state energies translates, through analytic continuation, to a corresponding excess phase shift in the scattering states [**?**].

## 14.12    Conclusion

Group theory entered physics it two distinct ways. On one level the set of transformations from one coordinate system (or observer) to another forms a group. Observers are related by the Galilean Principle of Relativity. On another level, some physical systems exhibit symmetry. This symmetry allows us to predict new states on the basis of states that are already observed, together with the application of some symmetry transformation. This is done through Einstein's Principle of Equivalence.

We have exploited these principles to describe the quantum mechanical properties, particularly the energy level structure, of hydrogenic atoms. Initially, we exploited a *geometric* symmetry, the symmetry of the Hamiltonian under rotations. The symmetry group is $SO(3)$ or the disconnected group $O(3)$. This symmetry requires that states occur in multiplets with angular momentum degeneracy $2l + 1$. It is surprising that hydrogenic states have a larger degeneracy than required by the rotation group $SO(3)$.

We believe that symmetry implies degeneracy, and the greater the symmetry, the greater the degeneracy. If we also believe that the $N^2$-fold degeneracy of the hydrogen states with principle quantum number $N$ is due to invariance under some group, we are prodded to search for a larger group $G \supset SO(3)$ that explains the $N^2$-fold degeneracy. This *dynamical* symmetry group is $SO(4)$: its six infinitesimal generators include both the angular momentum operators and the components of the Laplace-Runge-Lenz vector.

Why stop here? Why not search for a "symmetry" that breaks the degeneracy but maps any state of the hydrogen atom to linear combinations of all other states? Such *spectrum generating* groups include

$SO(4)$. The largest such group is the conformal group $SO(4,2)$. Before this group was discovered, the deSitter group $SO(4,1)$ was employed as a spectrum-generating group. A simple noncompact subgroup of these groups, isomorphic with $SO(2,1)$, was used to illustrate explicitly how the generators of a Lie algebra are used to determine eigenstates and energy eigenvalues. In addition, representations that describe bound states can be analytically continued to representations that describe scattering states. This analytic continuation relates bound state energies to phase shifts of scattering states. In the case that the Coulomb potential is perturbed by core shielding effects, the energy eigenvalue spectrum is often simply represented by a quantum defect that depends on the angular momentum. The phase shift of scattering states with angular momentum $l$ is related to the quantum defect with the same angular momentum.

In applications to the hydrogen atom, the role and scope of Group theory in physics is seen to extend far beyond applications depending on simple geometric symmetry.

## 14.13    Problems

1a.  **Principle of Relativity:** Assume two observers $S$ and $S'$ are locked the hold of a boat without windowports, so they cannot perceive the exterior world. Galilean Relativity is founded on two assumptions: (1) It is impossible to determine whether a noninertial frame is at rest or in relative motion with respect to its surroundings; (2) a body in an inertial frame will move with uniform velocity unless acted on by a force. Special Relativity is also founded on two assumptions: (1) the laws of physics are the same in all inertial frames; (2) the speed of light is the same in all inertial frames. The first of the Galilean assumptions is implicit in the Special Theory of Relativity. Show that the existence of the $3^{\text{deg}}$ microwave background radiation is incompatible with the first of Galileo's assumptions. Does this create a problem for the Special Theory of Relativity?

1b.  **Equivalence Principle:** Assume two observers $S$ and $S'$ are locked inside elevators without windows, so they cannot perceive the exterior world. Assume one elevator is sitting on the surface of the earth, so that the observer $S$ experiences a gravitational force $\mathbf{F} = m\mathbf{g}$ in the "down" direction. Assume that the other elevator is in "interstellar space" so that external gravitational forces "vanish", but that his

elevator experiences an acceleration **g** in the "up" direction. If the "rest of the universe" "looks the same" to both observers, argue that you can represent a gravitational field by a local acceleration. This use of the Equivalence Principle is one of the foundations of the General Theory of Relativity.

2. In the presence of a uniform magnetic field **B** show that the vector potential **A** can be taken as $\mathbf{A} = \frac{1}{2}\mathbf{B} \times \mathbf{r}$, so that $\mathbf{B} = \nabla \times \mathbf{A}$. Derive the Klein-Gordon equation for an electron in a Coulomb potential and a uniform magnetic field. Take the nonrelativistic limit of this and derive the Schrödinger equation for an electron in the presence of these two fields.

3. Make the ansatz $E = mc^2 + W$ in the Klein-Gordon equation and exhibit the terms in this equation that must be neglected in order to recover the nonrelativistic approximation, the Schrödinger equation.

4. Introduce spherical coordinates as follows: $(r, \theta, \phi) = (\theta_3, \theta_2, \theta_1)$ and

$$
\begin{aligned}
z = x_3 &= \theta_3 \cos \theta_2 \\
y = x_2 &= \theta_3 \sin \theta_2 \cos \theta_1 \\
x = x_1 &= \theta_3 \sin \theta_2 \sin \theta_1
\end{aligned}
$$

Show that $\mathcal{L}^2(S^1) = \partial^2/\partial\theta_1^2$. Show that

$$
\sin^2 \theta_2 \ \mathcal{L}^2(S^2) = \left( \sin \theta_2 \frac{\partial}{\partial \theta_2} \right)^2 + \mathcal{L}^2(S^1)
$$

Generalize this result to $\mathcal{L}^2(S^3)$ recursively using $\mathcal{L}^2(S^2)$ and $(\partial/\partial \cos \theta_3)^2$. Do this more generally for $\mathcal{L}^2(S^n)$.

5. This problem carries through the steps indicated in Table 14.1.

**a.** Show that the singular points of Eq. (14.9) occur at $r = 0$ and $r \to \infty$.

**b.** Show that in the neighborhood of the singular points

$$
\begin{array}{llll}
r \to 0 & \text{Eq.(14.9)} \to \left( \frac{d^2}{dr^2} + \frac{A}{r^2} \right) R(r) = 0 & R(r) \simeq r^\gamma & \gamma(\gamma - 1) + A = 0 \\
r \to \infty & \text{Eq.(14.9)} \to \left( \frac{d^2}{dr^2} + C \right) R(r) = 0 & R(r) \simeq e^{\lambda r} & \lambda^2 + C = 0
\end{array}
$$

Show that $\gamma = \frac{1}{2} \pm \sqrt{(\frac{1}{2})^2 - A}$ and $\lambda = \pm\sqrt{-C}$.

**c.** Show that if $\sqrt{(\frac{1}{2})^2 - A}$ is real, the solution with the positive sign is always square integrable in the neighborhood of $r = 0$. Under what conditions is the solution with the negative sign square integrable? Show that if $C < 0$ the solution $\pm\sqrt{-C}$ with the negative sign is square integrable. What happens if $C > 0$?

**d.** Show that a solution of the form $R(r) = r^\gamma e^{\lambda r} f(r)$ can be found where the function $f(r)$ is a simple polynomial function.

**e.** Find the equation that the function $f(r)$ satisfies. Show that it is equivalent to the equation given in Table 14.1.

**f.** Represent the function $f(r)$ as an ascending power series: $f(r) = \sum_{j=0}^{\infty} f_j \ r^j$. Find the two-term recursion relation satisfied by the coefficients $f_j$. Show that the recursion relation is

$$[(j+1)j + 2\gamma(j+1)] f_{j+1} + (2\lambda\gamma + 2\lambda j + B) f_j = 0$$

Use this relation to show

$$f(r) = \sum_{j=0} \frac{\Gamma(j + \gamma + (B/2\lambda))}{\Gamma(\gamma + (B/2\lambda))} \frac{\Gamma(2\gamma)}{\Gamma(j + 2\gamma)} \frac{(-2\lambda r)^j}{j!}$$

**g.** If this series does not terminate, show that its asymptotic behavior as $r \to \infty$, determined from the behavior of $f_j$ as $j \to \infty$, is $f(r) \to e^{-2\lambda r}$. Since $\lambda < 0$ this solution is not square integrable.

**h.** Conclude that the function $f(r)$ must be a polynomial of finite degree. If the highest nonzero degree term present is $r^n$, so that $f_n \neq 0$ but $f_{n+1} = 0$ ($\Rightarrow f_{n+2} = f_{n+3} = \cdots = 0$), show that the quantization conditon $2\lambda(n + \gamma) + B = 0$ must be satisfied. Show that this leads to the quantization condition in terms of the three parameters $A, B, C$ that appears in Eq.(14.9):

$$n + \frac{1}{2} + \sqrt{\left(\frac{1}{2}\right)^2 - A} = \frac{B}{2\sqrt{-C}}$$

**i.** Use the values of the parameters $A, B, C$ given in Eq.(14.10) to solve for the energy eigenvalues of the Klein-Gordon and Schrödinger equations:

$$E(n, l) = \frac{mc^2}{\sqrt{1 + \frac{\alpha^2}{(n + \frac{1}{2} + \sqrt{(l + \frac{1}{2})^2 - \alpha^2})^2}}} \qquad W(n, l) = -\frac{1}{2}mc^2\alpha^2 \frac{1}{(n + l + 1)^2}$$

Show that the polynomial solution is

$$f(r) = \sum_{j=0}^{n} \frac{\Gamma(2\gamma)}{\Gamma(j+2\gamma)} \frac{n!}{(n-j)!j!} (2\lambda r)^j$$

The radial part of the wavefunction $\frac{1}{r} r^\gamma f(r) e^{\lambda r}$ has exactly $n$ nodes in the open interval $(0, \infty)$.

6. For a highly ionized atom with $Z$ protons in its nucleus and a single remaining electron, show that the potential is $Ze/r$ and the solutions of the relativistic and nonrelativistic equations are obtained by the replacement $\alpha \to Z\alpha$. How large can $Z$ become before the relativistic solution is clearly incorrect? (Hint: set $l = 0$.)

7. Expand the relativistic energy in ascending powers of the fine structure constant to determine the relativistic corrections to the nonrelativistic energy. Show that, with $N' = n + \frac{1}{2} + \sqrt{\left(l + \frac{1}{2}\right)^2 - \alpha^2}$ and $N = n + l + 1$

$$E(n,l) = \frac{mc^2}{\sqrt{1 + \left(\frac{\alpha}{N'}\right)^2}} \to mc^2 - mc^2 \frac{1}{2N^2}\alpha^2 + mc^2 \left(\frac{3}{8N^4} - \frac{1}{N^3(2l+1)}\right)\alpha^4$$

$$+ mc^2 \left(-\frac{5}{16N^6} + \frac{3}{2N^5(2l+1)} - \frac{2N + 3(2l+1)}{2N^4(2l+1)^3}\right)\alpha^6 + mc^2 \times$$

$$\left(\frac{35}{128N^8} - \frac{15}{8N^7(2l+1)} + \frac{6N + 9(2l+1)}{4N^6(2l+1)^3} - \frac{2N^2 + 3N(2l+1) + 2(2l+1)^2}{N^5(2l+1)^5}\right)\alpha^8$$

$$+ \mathcal{O}(\alpha^{10})$$

8. The radial part of the wavefunction dies off like $e^{\lambda r}$ for large $r$, where $\lambda < 0$ for bound states. The parameter $\lambda$ has the dimensions of length, and $a \simeq 1/|\lambda|$ characterizes the size of a bound state orbit. Show that bound states with quantum numbers $(n, l)$ ($N = n + l + 1$ is the principal quantum number) have size scales

| | | |
|---|---|---|
| Relativistic | $a(n,l) = \sqrt{(N')^2 + \alpha^2}\, a_{\mathrm{B}}$ | $N' = n + \frac{1}{2} + \sqrt{\left(l + \frac{1}{2}\right)^2 - \alpha^2}$ |
| Nonrelativistic | $a(n,l) = N a_{\mathrm{B}}$ | $N = n + l + 1$ |

In these expressions $a_{\mathrm{B}} = \hbar^2/me^2 = 0.529 \times 10^{-8}$ cm is the Bohr radius:

Table 14.4. *Some particles that can be used to form hydreogen-like atoms.*

| Particle | Rest Energy (MeV) |
|---|---|
| electron $e^\pm$ | 0.511 |
| mu meson $\mu^\pm$ | 105.7 |
| tau meson $\tau^\pm$ | 1784. |
| proton, antiproton $p^\pm$ | 938.26 |
| deuteron $d^+$ | 1875.6 |
| tritium $t^+$ | 2809.4 |
| pi meson $\pi^\pm$ | 139.6 |
| sigma meson $\Sigma^\pm$ | 1385. |
| cascade meson $\Xi^-$ | 1533. |
| omega $\Omega^-$ | 1672. |

the characteristic size of the hydrogen atom in its ground state. By what percentage do the sizes of the atoms in the $(n, l)$ states differ between the relativistic and nonrelativistic treatments?

9. Many charged particles can form hydrogen-like atoms through their electrostatic interaction. Compute the energy spectrum for bound states of neutral atoms formed from a positively charged particle and a negatively charged particle drawn from this list of particles in Table 14.4. For each particle the mass is given in terms of the particle rest energy. Recall that the mass, $m$, that appears in the expression for the binding energy $W = -\frac{1}{2}mc^2\alpha^2/N^2$ is the reduced mass: $\frac{1}{m} = \frac{1}{m_1} + \frac{1}{m_2}$ of the two particles.

10. The motion of a classical nonrelativistic particle in a $1/r^2$ radial force field is a conic section: an elliptical orbit for bound states $(E < 0)$; hyperbolic for scattering states $(E > 0)$; and parabolic at the separatrix $(E = 0)$. If the radial force field includes a radial $1/r^3$ perturbation

$$f = -\frac{K}{r^2} + \frac{C}{r^3}$$

the trajectory has the form [42]

$$r = \frac{a(1 - \epsilon^2)}{1 + \epsilon\cos(\alpha\theta)}$$

where $\alpha = \sqrt{1 - \eta}, \eta = \frac{C}{Ka}$. This can be treated as an ellipse that is slowly rotating, $\alpha \simeq 1$. In this case the parameters $a$ and $\epsilon$ have their

usual meanings for elliptical orbits: $a$ is the semimajor axis and $\epsilon$ is the eccentricity. The ratio $\eta$ is a measure of the strength of the perturbation to the strength of the coulomb potential.

**a.** Expand the relativistic energy $E = \sqrt{(mc^2)^2 + (\mathbf{p}c)^2} - K/r$ to fourth order in $\mathbf{p}$ and show $E = (mc^2) + (p^2/2m) - (p^2/2m)^2/(2mc^2) - K/r = mc^2 + W$.

**b.** Replace the quartic term by $-(p^2/2m)^2/(2mc^2)$ by $-(W+K/r)^2/(2mc^2)$ and expand. Show that the classical hamiltonian for the motion of the (special) relativistic particle is

$$H = mc^2 + \frac{p^2}{2m} - \frac{K'}{r} + \frac{C'}{r^2}$$

Evaluate $K'$ and $C'$ and show $K' = K(1 + W/mc^2)$ and $C' = -K^2/(2mc^2)$.

**c.** Argue that the classical motion involves a renormalized coupling $K \rightarrow K'$ as well as a $1/r^3$ component to the force, with $C = 2C'$.

**d.** Show that the advance in the perihelion of the orbit is $\delta\theta \simeq \eta/2$ per period.

**e.** Evaluate $\eta$ for the planet Mercury, for which $\epsilon = 0.206$ and the period is $T = 0.24$ year. Show that this amounts to about 7" per century. The general relativistic correction is larger by a factor of 6, and accounts for the observed advance in Mercury's perihelion of 42"/century.

**f.** The existence of precessing elliptical orbits is due to the "relativistic mass velocity" correction. This can be viewed from two perspectives. (1) Newton's equations are correct and the mass of the particle varies with its state of motion according to $m = m_0/\sqrt{1 - (v/c)^2}$. (2) The mass of a particle is a constant of Nature and Newton's (nonrelativistic) equations of motion are not correct for relativistic particles, and must be modified. The author feels the second interperetation is far superior to the first.

11. When the attracting potential is central and nearly $1/r$, the motion of a bound particle is nearly elliptical. It is useful to describe this motion as if it were elliptical, with the semimajor axis of the ellipse precessing in the plane of motion. Assume that the force has the form $\mathbf{F}(r) = (-K/r^2 + p(r))\hat{\mathbf{r}}$, where $p(r)$ is a small perturbation. The rate

at which the Runge-Lenz vector precesses is

$$\omega = \frac{\partial}{\partial L}\left(\frac{1}{T}\int p(r)\ dt\right) = \frac{\partial}{\partial L}\left(\frac{m}{LT}\oint r^2 p(r)\ d\theta\right)$$

with $1/r = \frac{mK}{L^2}(1 + \frac{M}{mK}\cos\theta)$. Here $L$ is the particle's orbital angular momentum and $T$ is its period. If the perturbing term is of the form $C/r^3$ the integral is $C \times 2\pi\frac{mK}{L^2}$. The perturbations due to Special and General Relativity are

Special Relativity     $C = \dfrac{KL^2}{2m^2c^2}$     $\omega = \dfrac{\pi K^2}{TL^2c^2}$

General Relativity     $C = 6 \times \dfrac{KL^2}{2m^2c^2}$     $\omega = \dfrac{6\pi K^2}{TL^2c^2}$

For planetary motion $K = GMm$. When $M \gg m$, $\omega$ is (almost) independent of $m$. Why? Determine how the relativistic precession $\omega$ scales (cf. Problem 16.3, last chapter) with planetary distance from the sun. What is the precession for the earth? Use $\omega = 42''/\text{cent}$ for Mercury and the following distance ratios:

| Mercury | Venus | Earth | Mars | Jupiter | Saturn | Uranus | Neptune |
|---------|-------|-------|------|---------|--------|--------|---------|
| 0.39 | 0.72 | 1.00 | 1.52 | 5.20 | 9.54 | 19.18 | 30.06 |

12. The action of the angular momentum shift down operator $L_-$ on the lowest $m$-value spherical harmonic for a given value of $l$ is zero: $L_-Y^l_{m=-l}(\theta,\phi) = 0$. Use the coordinate representation for $L_-$ to compute this function.

**a.** Write $Y^l_m(\theta,\phi) = P^l_{-l}(\theta)e^{-il\phi}$ and show

$$\left(-\frac{\partial}{\partial\theta} + i\frac{\cos\theta}{\sin\theta}\frac{\partial}{\partial\phi}\right)P^l_{-l}(\theta)e^{-il\phi} = e^{-il\phi}\left(-\frac{\partial}{\partial\theta} + l\frac{\cos\theta}{\sin\theta}\frac{\partial}{\partial\phi}\right)P^l_{-l}(\theta)$$

**b.** Show $P^l_{-l} = (\sin\theta)^l$ satisfies this equation.
**c.** This function is not normalized to unity over the sphere. Normalize it by introducing a normalization coefficient $N_l$ and enforcing the condition

$$\int_0^\pi d\theta\ \sin\theta \int_0^{2\pi} d\phi|N_l \sin^l\theta e^{-il\phi}|^2 = 1$$

**d.** Show that $N_l = \sqrt{\frac{1}{4\pi}}\sqrt{\frac{(2l+1)!!}{(2l)!!}}$.

**e.** This leads the the simple recursion relation for normalization coeffi-
cients for the $Y^l_{\pm l}(\theta, \phi)$:

$$N_l = \sqrt{\frac{2l+1}{2l}}\, N_{l-1}$$

Compare these results with Table 14.2 using initial condition
$N_0 = \sqrt{\frac{1}{4\pi}}$. Compute $N_3$.

**f.** Use the numerical value of the matrix elements $\langle \begin{smallmatrix} l \\ m' \end{smallmatrix} |L_+| \begin{smallmatrix} l \\ m \end{smallmatrix} \rangle = \sqrt{(l+m')(l-m)}\, \delta_{m',m+1}$ and the coordinate representation of
the shift up operator $L_+$ to construct the correctly normalized
spherical harmonics $Y^l_m(\theta, \phi)$.

13. Use methods similar to those described in Problem 12 to construct
the radial wavefunctions for hydrogenic atoms with extreme orbital an-
gular momentum quantum numbers: $l = N - 1$, where in general the
principle quantum number $N = n+l+1$. These functions have no nodes
in the interval $(0, \infty)$ (since $n = 0$).

14. Show $\dfrac{d}{dt}\left(\dfrac{\mathbf{r}}{r}\right) = \dfrac{\dot{\mathbf{r}}(\mathbf{r}\cdot\mathbf{r}) - \mathbf{r}(\mathbf{r}\cdot\dot{\mathbf{r}})}{r^3} = -\dfrac{\mathbf{r}\times(\mathbf{r}\times\dot{\mathbf{r}})}{r^3}.$

15. $\mathbf{r}$ is the position vector from the sun to a planet, or from the
proton to the electron in the hydrogen atom, $\mathbf{L} = \mathbf{r}\times\mathbf{p}$ is the orbital
angular momentum, and $\mathbf{M}$ is the Laplace-Runge-Lenz vector.

**a.** $\mathbf{M}\cdot\mathbf{L} = 0$.
**b.** $\mathbf{M}\cdot\mathbf{M} = \frac{2\mathbf{L}\cdot\mathbf{L}}{m}\left(\frac{\mathbf{p}\cdot\mathbf{p}}{2m} - \frac{K}{r}\right) + K^2$.
**c.** $\mathbf{M}\cdot\mathbf{r} = \frac{\mathbf{L}\cdot\mathbf{L}}{m} - Kr$.
**d.** $\mathbf{M}\cdot\mathbf{r} = Mr\cos\theta$.
**e.** $r = \frac{\mathbf{L}\cdot\mathbf{L}/mK}{1+(M/K)\cos\theta}$.
**f.** Compare this result to the standard solution of the trajectory equa-
tions for motion in a $1/r$ potential to conclude: $L^2/mK$ is the
semimajor axis of the elliptical orbit and $\epsilon = M/K$ is the ec-
centricity of the orbit.
**g.** Conclude that the Laplace-Runge-Lenz vector is a constant of motion
that points to the perihelion of the elliptical orbit.

16. Show that $\mathbf{A}\cdot\mathbf{A} = \frac{-1}{4\hbar^2}(\mathbf{L}\cdot\mathbf{L} + \mathbf{M}'\cdot\mathbf{M}' + \mathbf{L}\cdot\mathbf{M}' + \mathbf{M}'\cdot\mathbf{L})$. Show
that $\mathbf{B}\cdot\mathbf{B}$ has a similar expression. Show that the two expressions are
equal since $\mathbf{L}\cdot\mathbf{M} = \mathbf{M}\cdot\mathbf{L} = 0$.

17. Show that the inverse of the stereographic projection given in eq.(14.35) is

$$\frac{\mathbf{p}}{p_0} = \frac{\mathbf{u}}{1 - \mathbf{u} \cdot \mathbf{w}}$$

18. Compute $p_x = \mathbf{p} \cdot \mathbf{M}/M$ and $p_y = \mathbf{p} \cdot \mathbf{W}/W$. Show $p_x^2 + (p_y - a)^2 = r^2$. Explicitly compute the displacement vector $a$ (i.e., $(0, a)$) and the radius $r$ of circular motion. Show that circles in $R^3$ lift to circles in $S^3 \subset R^4$ under the stereographic projection of Eq.(14.35). Show that circles in $S^3$ project back down to circles in $R^3$ under the inverse transformation.

19. Show that the number of independent monomials of the form $x^a y^b z^c$, with $a, b, c$ nonnegative integers and $a + b + c = l$ is $N(l, 3) = (l + 3 - 1)/l!(3 - 1)!$. In $N$-dimensional space show that the number of homogeneous polynomials of degree $l$ in $x_1, x_2, \ldots x_N$ is obtained by replacing $3 \to N$ in this expression. This is the *Bose-Einstein counting* statistic.

**a.** Show that the functions $r^l Y_m^l(\theta, \phi)$ are homogeneous polynomials in $x, y, z$ of degree $l$.

**b.** Show that the number of independent spherical harmonics of degree $l$ is the difference between the number of homogeneous polynomials of degree $l$ and $l - 2$ on three variables: $dim\{Y_m^l\} = N(l, 3) - N(l - 2, 3) = 2l + 1$.

**c.** After stereographic transformation into four dimensions, the hydrogen wavefunctions in the momentum representation are spherical harmonics in four variables [3]. Show that the number of spherical harmonics of degree $n$ is $dim\{\mathcal{Y}_{lm}^n\} = N(n, 4) - N(n - 2, 4) = (n + 1)^2$.

**d.** Construct homogeneous polynomials of degree $0, 1, 2$ and the spherical harmonics associated with these homogeneous polynomials. Take the inverse Fourier transform of these spherical harmonics to obtain the hydrogen atom wavefucntions $\psi(\mathbf{x})_{nlm}$ for $n = 0, 1, 2$; $l = 0, \ldots, n - 1$; and $-l \leq m \leq +l$.

**e.** Show that the recursive relation used to build up a Pascal triangle can be written in the symmetric form

$$\frac{(a + b + 1)!}{(a + \frac{1}{2})!(b + \frac{1}{2})!} = \frac{(a + b)!}{(a - \frac{1}{2})!(b + \frac{1}{2})!} + \frac{(a + b)!}{(a + \frac{1}{2})!(b - \frac{1}{2})!}$$

where $a$ and $b$ are half odd integers: $\frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \ldots$ .

**f.** Show homogeneous polynomials satisfy the recursion relation:$N(l,d) = N(l,d-1) + N(l-1,d)$.

**g.** Use this result to derive the following recursion relation for the dimensions of the spaces of spherical harmonics on spheres $S^n$ and $S^{n-1}$:

$$\dim \mathcal{Y}^l(S^n) = \dim \mathcal{Y}^{l-1}(S^n) + \dim \mathcal{Y}^l(S^{n-1})$$

For the case $n = 3$ this gives $(l+1)^2 = l^2 + (2l+1)$. The initialization for all $n$ is $\mathcal{Y}^0(S^n) = 1 = \dim \mathcal{Y}^0(S^n)$.

**h.** $\dim \mathcal{Y}^l(S^n) = \frac{(l+n-2)!}{l!(n-1)!}(2l+n-1)$.

20. **$D$-Dimensional Coulomb Problem:** In $D$-dimensional space the Schrödinger equation for the Kepler problem is Eq. (14.4) in the relativistic case and Eq. (14.5) in the nonrelativistic case. The only difference is that the Laplacian $\nabla^2$ is on $D$ coordinates rather than three. In this case the Laplacian operator is

$$\nabla^2 = \left(\frac{1}{r^{D-1/2}}\frac{\partial}{\partial r} r^{D-1/2}\right)^2 + \frac{\mathcal{L}^2}{r^2}$$

The angular part of the Laplacian operator, $\mathcal{L}^2$, acts on spherical harmonics on $S^{D-1}$, $\mathcal{Y}^l(S^{D-1})$. These spherical harmonics are eigenfunctions of this (Laplace-Beltrami) operator with eigenvalue $-[(l+\alpha)^2 - \alpha^2]$, and $\alpha$ is a quantity that depends on the Lie algebra of $SO(D)$: it is half the sum over all positive roots of the algebra. For the Lie algebras of the orthogonal roots the coefficient of the sum that is important is $\alpha = D-2$.

**a.** Show that $\psi(\mathbf{x}) = \frac{1}{r^{(D-1)/2}}\mathcal{Y}^l(\text{angles})$ is a clever ansatz that reduces the Schrödinger equation in $D$ dimensions to the form of Eq. (14.4) in the relativistic case and Eq. (14.5) in the nonrelativistic case.

**b.** Show that the only change in Eq.(14.10) is the replacement $(l+\frac{1}{2})^2 - (\frac{1}{2})^2 \to (l+\frac{D-2}{2})^2 - (\frac{D-2}{2})^2$ in column A.

**c.** Show that the relativistic and nonrelativistic energies shown in Eq.(14.12) change as follows:

Relativistic $\quad N' \to n+\frac{1}{2}+\sqrt{(l+\frac{1}{2})^2+l(D-3)-\alpha^2}$

Non Relativistic $\quad N \to n+\frac{1}{2}+\sqrt{(l+\frac{1}{2})^2+l(D-3)}$

21. Compute the quantum defect in heavy atoms by using the Klein-Gordon equation and a $-1/r^2$ perturbation. Show that the bound state

energy and scattering phase shifts are given by the substitution $l(l+1) \rightarrow l(l+1) - \mu_l$. Argue that electrons in the $s$ state penetrate the core much more deeply (on average) and $p$-state electrons (than $d$-state electrons, ...) so that $\mu_0 \gg \mu_1 > \cdots$.

22. The isotropic harmonic oscillator in $n$ dimensions has hamiltonian

$$H = \sum_{i=1}^{n} \hbar\omega \left( a_i^\dagger a_i + \frac{1}{2} \right)$$

**a.** Show that the Lie algebra of its geometric symmetry group is spanned
  by the angular momentum operators $L_{ij} = a_i^\dagger a_j - a_j^\dagger a_i = -L_{ji}$.

**b.** Show that the Lie algebra of its dynamical symmetry group is spanned
  by the angular momentum operators together with the quadrupole
  tensor operators $Q_{ij} = a_i^\dagger a_j + a_j^\dagger a_i = +Q_{ji}$.

**c.** Show that one spectrum generating algebra includes the operators
  $\mathbf{L}$ and $\mathbf{Q}$ as well as the single boson operators $a_i^\dagger$ and $a_j$, as
  well as their commutator $[a_i, a_j^\dagger] = 1$. Show that this algebra is
  nonsemisimple and describe its structure.

**d.** Show that another spectrum generating algebra consists of the op-
  erators $\mathbf{L}$ and $\mathbf{Q}$ as well as the two boson creation operators
  $a_i^\dagger a_j^\dagger$ and two boson annihilation operators $a_i a_j$. Show that this
  algebra is simple and describe its structure. Show that this
  spectrum generating algebra does not couple all the states that
  exist: "parity" is an invariant, where "parity" is even or odd
  according to whether the number of excitations in the spectrum
  is even or odd.