9. Group Theory of the Hydrogen Atom and the Kepler Problem

The hydrogen atom has the Hamiltonian

$$H = \frac{p^2}{2\mu} - \frac{e^2}{4\pi\epsilon_0}\frac{1}{r}, \qquad 9.1$$

where the Coulomb attraction between the proton and the electron is expressed in SI units. This is a central force problem (cf. Section 8. -- "Central Force Problems and Angular Momentum") and the central force is

$$F(r) = \frac{k}{r^2}, \qquad k = \frac{-e^2}{4\pi\epsilon_0}. \qquad 9.2$$

Thus, the hydrogen atom is an example of the Kepler problem. Consequently, it possesses symmetry additional to that arising from its rotational symmetry (which results in conservation of angular momentum). This additional symmetry is described below in group theoretical terms, following some classical mechanical details of the Kepler problem.

The Classical Kepler Problem

The Kepler problem is a two-body central force problem with $F(r) = k/r^2$. Angular momentum, $\vec{L} = \vec{r} \times \vec{p}$, is conserved in this problem. The vector quantity

$$\vec{A} \equiv \vec{L} \times \frac{d\vec{r}}{dt} - k\frac{\vec{r}}{r} \qquad 9.3$$

is also conserved in this problem:

Theorem 9.1

$$\frac{d\vec{A}}{dt} = \frac{d}{dt}\left\{ \vec{L} \times \frac{d\vec{r}}{dt} - k\frac{\vec{r}}{r} \right\} = 0. \qquad 9.4$$

Consider

$$\vec{L} \times \frac{d^2\vec{r}}{dt^2} = \frac{F(r)}{\mu r} \vec{L} \times \vec{r},$$

where eq. (8.5) has been used. Then, using the identity

$$(\vec{A} \times \vec{B}) \times \vec{C} = (\vec{A} \cdot \vec{C})\vec{B} - \vec{A}(\vec{B} \cdot \vec{C})$$

it follows that for

$$\vec{L} \times \vec{r} = \left\{ \vec{r} \times \mu \frac{d\vec{r}}{dt} \right\} \times \vec{r},$$

$$\vec{L} \times \vec{r} = r^2 \mu \frac{d\vec{r}}{dt} - \vec{r} \left\{ \mu \frac{d\vec{r}}{dt} \cdot \vec{r} \right\}.$$

$$\therefore \quad \vec{L} \times \vec{r} = r^2 \mu \frac{d\vec{r}}{dt} - \vec{r} \mu \frac{dr}{dt} r,$$

$$\therefore \quad \vec{L} \times \vec{r} = \mu r^3 \frac{d}{dt}\left(\frac{\vec{r}}{r}\right),$$

$$\therefore \quad \vec{L} \times \frac{d^2\vec{r}}{dt^2} = F(r)\, r^2 \frac{d}{dt}\left(\frac{\vec{r}}{r}\right).$$

Then for

$$F(r) = \frac{k}{r^2},$$

$$\vec{L} \times \frac{d^2\vec{r}}{dt^2} = k \frac{d}{dt}\left(\frac{\vec{r}}{r}\right);$$

or rearranging and using eq. (8.8),

$$\frac{d}{dt}\left\{ \vec{L} \times \frac{d\vec{r}}{dt} - k\frac{\vec{r}}{r} \right\} = 0.$$

$$\therefore \frac{d\vec{A}}{dt} = 0$$

Q.E.D.

The vector $\vec{A}$ is the <u>Laplace - Runge - Lenz vector</u> or <u>Lenz vector</u> (for short).

The Lenz vector has a number of properties that illuminate the structure of the Kepler problem:

(i). $\vec{A}\cdot\vec{L} = \left(\vec{L}\times\frac{d\vec{r}}{dt}\right)\cdot\vec{L} - k\frac{\vec{r}}{r}\cdot\left(\vec{r}\times\mu\frac{d\vec{r}}{dt}\right),$

$$\therefore \vec{A}\cdot\vec{L} = 0. \qquad 9.5$$

(Recall $\vec{A}\cdot(\vec{A}\times\vec{B}) = (\vec{A}\times\vec{B})\cdot\vec{A} = 0.$)

Thus, the Lenz vector is perpendicular to the orbital angular momentum vector, i.e. it lies in the orbital plane.

(ii). $\vec{A}\cdot\vec{r} = \left(\vec{L}\times\frac{d\vec{r}}{dt}\right)\cdot\vec{r} - k\frac{\vec{r}}{r}\cdot\vec{r},$

$$\therefore \vec{A}\cdot\vec{r} = \left\{\left(\vec{r}\times\mu\frac{d\vec{r}}{dt}\right)\times\frac{d\vec{r}}{dt}\right\}\cdot\vec{r} - \frac{kr^2}{r};$$

and using the identity

$$(\vec{A}\times\vec{B})\times\vec{C} = (\vec{A}\cdot\vec{C})\vec{B} - \vec{A}(\vec{B}\cdot\vec{C}),$$

$$\therefore \vec{A}\cdot\vec{r} = \left(\vec{r}\cdot\frac{d\vec{r}}{dt}\right)\mu\frac{d\vec{r}}{dt}\cdot\vec{r} - (\vec{r}\cdot\vec{r})\left(\mu\frac{d\vec{r}}{dt}\cdot\frac{d\vec{r}}{dt}\right) - kr.$$

$$\therefore \vec{A}\cdot\vec{r} = \mu\left(\vec{r}\cdot\frac{d\vec{r}}{dt}\right)^2 - \mu r^2\frac{d\vec{r}}{dt}\cdot\frac{d\vec{r}}{dt} - kr.$$

Then, defining $\vec{p} = \mu\, d\vec{r}/dt$,

$$\vec{A}\cdot\vec{r} = \frac{(\vec{r}\cdot\vec{p})^2}{\mu} - \frac{r^2p^2}{\mu} - kr;$$

and using the identity

$$(\vec{A}\times\vec{B})\cdot(\vec{A}\times\vec{B}) = A^2B^2 - (\vec{A}\cdot\vec{B})^2,$$

and $\vec{L} = \vec{r}\times\vec{p}$,

$$\vec{A}\cdot\vec{r} = -\frac{L^2}{\mu} - kr.$$

But

$$\vec{A}\cdot\vec{r} = Ar\cos\theta,$$

whence

$$r = \frac{L^2}{-k\mu(1+\varepsilon\cos\theta)}, \qquad 9.6$$

where $\varepsilon \equiv A/k$. This is the classical orbit equation. The magnitude of the Lenz vector is proportional to the eccentricity of the orbit.

(iii). Properties (i) and (ii) can be combined to produce a simple picture of Kepler orbits. The case $k<0$, i.e. for bound states, is shown in fig. 9.1. The Lenz vector

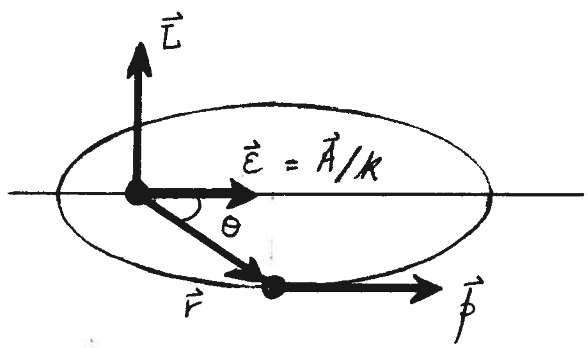

Fig. 9.1 The relationship between $\vec{r}$, $\vec{p} = \mu d\vec{r}/dt$, $\vec{L} = \vec{r}\times\vec{p}$, and $\vec{\varepsilon} = \vec{L}\times\vec{p}/\mu k - \vec{r}/r = \vec{A}/k$ in the Kepler problem.

is directed along the major axis of an elliptical orbit as shown in fig. 9.1. The geometry of the elliptical orbit is shown in fig. 9.2. The eccentricity, $\varepsilon = A/k$, and

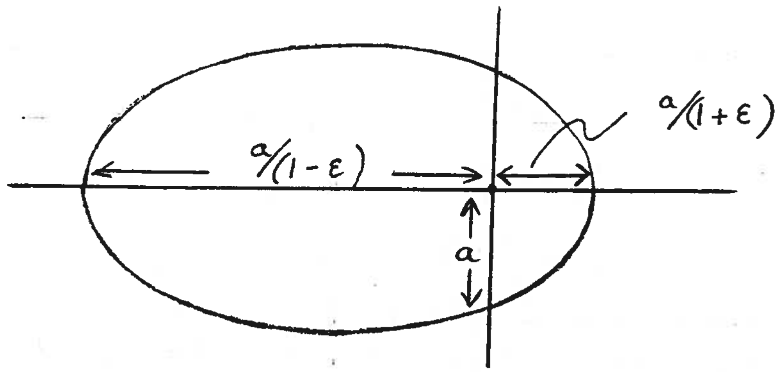

Fig. 9.2. The geometry of an elliptical orbit in the Kepler problem. The eccentricity is ε; the semi-latus rectum is $a = L^2/(-k\mu)$.

the semi-latus rectum, $a = L^2/(-k\mu)$, do not change with time: the elliptical orbits of the Kepler problem do not precess.

(iv). $$\vec{A}\cdot\vec{A} = \left(\frac{\vec{L}\times\vec{p}}{\mu} - k\frac{\vec{r}}{r}\right)\cdot\left(\frac{\vec{L}\times\vec{p}}{\mu} - k\frac{\vec{r}}{r}\right),$$

$$\therefore \vec{A}\cdot\vec{A} = \frac{(\vec{L}\times\vec{p})\cdot(\vec{L}\times\vec{p})}{\mu^2} - 2k\frac{(\vec{L}\times\vec{p})\cdot\vec{r}}{\mu r} + k^2\frac{\vec{r}\cdot\vec{r}}{r^2},$$

and using the identity

$$(\vec{A}\times\vec{B})\cdot(\vec{A}\times\vec{B}) = A^2B^2 - (\vec{A}\cdot\vec{B})^2,$$

then

$$(\vec{L}\times\vec{p})\cdot(\vec{L}\times\vec{p}) = L^2p^2 - \cancel{(\vec{L}\cdot\vec{p})^2}^{\,0},$$

and, from (ii)

$$(\vec{L}\times\vec{p})\cdot\vec{r} = -L^2,$$

whence

$$\vec{A}\cdot\vec{A} = \frac{2kL^2}{\mu r} + \frac{L^2 p^2}{\mu^2} + k^2,$$

and, from $\vec{\varepsilon} = \vec{A}/k$

$$\vec{\varepsilon}\cdot\vec{\varepsilon} = \frac{2L^2}{\mu k r} + \frac{L^2 p^2}{k^2\mu^2} + 1 .$$

$$\therefore \quad \varepsilon^2 = 1 + \frac{2L^2}{k^2\mu}\left(\frac{p^2}{2\mu} + \frac{k}{r}\right),$$

$$\therefore \quad \varepsilon^2 = 1 + \frac{2L^2}{k^2\mu} H . \qquad 9.7$$

(Since L^2 and H are conserved quantities, the magnitude of the Lenz vector is seen again to be a conserved quantity.)

Then, defining

$$K^2 = -\frac{k^2\mu}{2H}\varepsilon^2, \qquad 9.8$$

the Hamiltonian can be written as

$$H = \frac{-k^2\mu}{2}\frac{1}{K^2+L^2} . \qquad 9.9$$

From fig. 9.2, the length of the major axis of the elliptical orbit, Λ, is

$$\Lambda = \frac{a}{1-\varepsilon} + \frac{a}{1+\varepsilon} = \frac{2a}{1-\varepsilon^2} = \frac{2L^2}{(-k)\mu(1-\varepsilon^2)} ;$$

and thus from eq. (9.7)

$$1-\varepsilon^2 = -2\frac{L^2 H}{k^2\mu} .$$

$$\therefore \quad \Lambda = \frac{k}{H} \qquad 9.10$$

The Quantum Kepler Problem (Hydrogen Atom)

The Hamiltonian for the quantum Kepler problem is

$$H = \frac{p^2}{2\mu} + \frac{k}{r}. \qquad 9.11$$

Besides possessing L^2 and L_z as simultaneous observables to H, operators associated with the Lenz vector -- A_x, A_y, A_z, and A^2 -- obey the following relationships:

$$[H, A_x] = [H, A_y] = [H, A_z] = [H, A^2] = 0, \qquad 9.12$$

$$\vec{L}\cdot\vec{A} = \vec{A}\cdot\vec{L} = 0, \qquad 9.13$$

$$[L_x, A_x] = 0, \quad [L_x, A_y] = i\hbar A_z, \quad [L_x, A_z] = -i\hbar A_y, \qquad 9.14$$

$$[L_y, A_x] = -i\hbar A_z, \quad [L_y, A_y] = 0, \quad [L_y, A_z] = i\hbar A_x, \qquad 9.15$$

$$[L_z, A_x] = i\hbar A_y, \quad [L_z, A_y] = -i\hbar A_x, \quad [L_z, A_z] = 0; \qquad 9.16$$

and for the "rescaled" Lenz vector:

$$\vec{K} = \sqrt{\frac{\mu}{-2H}}\,\vec{A} = \sqrt{\frac{\mu}{-2E}}\,\vec{A}, \qquad 9.17$$

where $E < 0$ for the bound Kepler problem,

$$[K_x, K_y] = i\hbar L_z, \quad [K_y, K_z] = i\hbar L_x, \quad [K_z, K_x] = i\hbar L_y, \qquad 9.18$$

and

$$H = -\frac{k^2\mu}{2}\,\frac{1}{K^2 + L^2 + \hbar^2} \qquad 9.19$$

(cf. eqs. (9.19) and (9.9)).

(Here, $\hbar$ is retained explicitly to show where it appears in these less familiar relations.) The quantum mechanical (operator) form of $\vec{A}$ is

$$\vec{A} = \frac{1}{2\mu}\left(\vec{L}\times\vec{p} - \vec{p}\times\vec{L}\right) - \frac{k\vec{r}}{r}, \qquad 9.20$$

the "symmetrized" form being necessary because $\vec{L}$ and $\vec{p}$ do not commute. This form must be postulated (as an axiom) in order to obtain the correct quantum mechanical results, and it is called the <u>Pauli-Lenz vector.</u>

The derivations of eqs. (9.12-19) involve laborious manipulations of commutator bracket algebra: these are carried through in detail. The form of $\vec{A}$ chosen for this is

$$\vec{A} = \frac{1}{\mu}\left\{\vec{p}(\vec{r}\cdot\vec{p}) - \vec{r}p^2 - \mu\frac{k\vec{r}}{r}\right\}. \qquad 9.21$$

Equation (9.21) is derived in the Appendix to this section (eq. (9A.31)).

(i). To show that $[H, A_x] = 0$: ($x, y, z \rightarrow 1, 2, 3$ is used here)

$$[H, A_1] = \frac{1}{\mu}\left\{\frac{1}{2\mu}[p^2, p_1(\vec{r}\cdot\vec{p})] + k[r^{-1}, p_1(\vec{r}\cdot\vec{p})] - \frac{1}{2\mu}[p^2, r_1p^2] - k[r^{-1}, r_1p^2] - \frac{k}{2}[p^2, r_1r^{-1}]\right\}$$

$$
\begin{aligned}
\therefore [H, A_1] = \frac{1}{\mu}\Big\{ & \frac{1}{2\mu} p_1 [p^2, (\vec{r}\cdot\vec{p})] && = \frac{1}{\mu}\Big\{ \cancel{\frac{1}{2\mu} p_1 (-2i\hbar p^2)} \\
& + k\, p_1 [r^{-1}, (\vec{r}\cdot\vec{p})] && \cancel{+ k p_1 (-i\hbar r^{-1})} \\
& + k [r^{-1}, p_1](\vec{r}\cdot\vec{p}) && + k(-i\hbar r_1 r^{-3})(\vec{r}\cdot\vec{p}) \\
& - \frac{1}{2\mu}[p^2, r_1] p^2 && \cancel{- \frac{1}{2\mu}(-2i\hbar p_1) p^2} \\
& - k\, r_1 [r^{-1}, p^2] && \times \tfrac{1}{2} \quad - k r_1 \left(-i\hbar(\vec{p}\cdot\vec{r}) r^{-3} - i\hbar r^{-3}(\vec{r}\cdot\vec{p})\right) \\
& - \frac{k}{2} r_1 [p^2, r^{-1}] && - \frac{k}{2} r_1 \left(i\hbar(\vec{p}\cdot\vec{r}) r^{-3} \cancel{+ i\hbar r^{-3}(\vec{r}\cdot\vec{p})}\right) \\
& - \frac{k}{2}[p^2, r_1] r^{-1} \Big\} && \cancel{- \frac{k}{2}(-2i\hbar p_1) r^{-1}} \Big\}
\end{aligned}
$$

$$\therefore [H, A_1] = \frac{i\hbar k}{\mu}\left\{ -\tfrac{1}{2} r_1 r^{-3}(\vec{r}\cdot\vec{p}) + \frac{1}{2} r_1 (\vec{p}\cdot\vec{r}) r^{-3} \cancel{+ \frac{1}{2} r_1 r^{-3}(\vec{r}\cdot\vec{p})} \right\}$$

$$= \frac{i\hbar k}{\mu}\left\{ -\frac{1}{2} r_1 r^{-3}(\vec{r}\cdot\vec{p}) + \frac{1}{2} r_1 \left((\vec{r}\cdot\vec{p}) - 3i\hbar\right) r^{-3} \right\}$$

$$= \frac{i\hbar k}{2\mu} r_1 \left\{ [(\vec{r}\cdot\vec{p}), r^{-3}] - 3i\hbar\, r^{-3} \right\}$$

$$\therefore [H, A_1] = 0$$

$[H, A_2] = [H, A_3] = 0$ follow from the isotropy of the problem, whence $[H, A^2] = 0$, so yielding eq. (9.12).

(ii). To show that $\vec{L}\cdot\vec{A} = 0$.

$$\vec{L}\cdot\vec{A} = \frac{1}{\mu}\left\{(\vec{L}\cdot\vec{p})(\vec{r}\cdot\vec{p}) - (\vec{L}\cdot\vec{r})p^2 - \frac{\mu k}{r}(\vec{L}\cdot\vec{r})\right\}.$$

Caution is needed in arguing that

$\vec{L}\cdot\vec{p} = (\vec{r}\times\vec{p})\cdot\vec{p} = 0$,

$\vec{L}\cdot\vec{r} = (\vec{r}\times\vec{p})\cdot\vec{r} = 0$,

because $\vec{p}$ and $\vec{r}$ are not sharply defined. However,

$$(\vec{r}\times\vec{p})\cdot\vec{p} = (r_2p_3 - r_3p_2)p_1 + (r_3p_1 - r_1p_3)p_2 + (r_1p_2 - r_2p_1)p_3\,,$$

and since each term contains fully commuting quantities, then indeed $\vec{L}\cdot\vec{p} = 0$; and similarly $\vec{L}\cdot\vec{r} = 0$.

$\therefore\ \vec{L}\cdot\vec{A} = 0$, and hence $\vec{A}\cdot\vec{L} = 0$, so yielding eq. (9.13).

(iii). To show that $[L_i, A_j] = i\hbar\,\varepsilon_{ijk}A_k$, $i,j,k = 1,2,3$.

$\vec{A}$ is a vector operator and thus obeys the general result for any vector operator $\vec{V}$ (eqs. (7.104 – 112). Thus, eqs. (9.14-16) follow directly.

(iv). To show that $[K_i, K_j] = i\hbar\,\varepsilon_{ijk}L_k$, $i,j,k = 1,2,3$.

Consider $[A_1, A_2]$ with $A_1 = \mu^{-1}\{p_1(\vec{r}\cdot\vec{p}) - r_1p^2 - \mu k r_1 r^{-1}\}$ and

---

Recall $\varepsilon_{ijk} = \varepsilon_{jki} = \varepsilon_{kij} = +1$, $\varepsilon_{jik} = \varepsilon_{ikj} = \varepsilon_{kji} = -1$,
$\varepsilon_{iij} = 0$.

$$A_2 = \mu^{-1}\left\{ p_2 (\vec{r}\cdot\vec{p}) - r_2 p^2 - \mu k\, r_2 r^{-1} \right\}.$$

$$\begin{aligned}
\therefore [A_1, A_2] = \mu^{-2}\Big\{ & [p_1(\vec{r}\cdot\vec{p}), p_2(\vec{r}\cdot\vec{p})] - [p_1(\vec{r}\cdot\vec{p}), r_2 p^2] - \mu k [p_1(\vec{r}\cdot\vec{p}), r_2 r^{-1}] \\
& - [r_1 p^2, p_2(\vec{r}\cdot\vec{p})] + [r_1 p^2, r_2 p^2] + \mu k [r_1 p^2, r_2 r^{-1}] \\
& - \mu k [r_1 r^{-1}, p_2(\vec{r}\cdot\vec{p})] + \mu k [r_1 r^{-1}, r_2 p^2] \Big\},
\end{aligned}$$

[cancellations]

$$\begin{aligned}
\therefore [A_1, A_2] = \mu^{-2}\Big\{ & p_1 [(\vec{r}\cdot\vec{p}), p_2](\vec{r}\cdot\vec{p}) \\
& + p_2 [p_1, (\vec{r}\cdot\vec{p})](\vec{r}\cdot\vec{p}) \\
& - p_1 [(\vec{r}\cdot\vec{p}), r_2] p^2 \\
& - p_1 r_2 [(\vec{r}\cdot\vec{p}), p^2] \\
& - \mu k\, p_1 [(\vec{r}\cdot\vec{p}), r_2] r^{-1} \\
& - \mu k\, p_1 r_2 [(\vec{r}\cdot\vec{p}), r^{-1}] \\
& - \mu k\, r_2 [p_1, r^{-1}](\vec{r}\cdot\vec{p}) \\
& - r_1 p_2 [p^2, (\vec{r}\cdot\vec{p})] \\
& - p_2 [r_1, (\vec{r}\cdot\vec{p})] p^2 \\
& + r_1 [p^2, r_2] p^2 \\
& + r_2 [r_1, p^2] p^2 \\
& + \mu k\, r_1 [p^2, r_2] r^{-1} \\
& + \mu k\, r_1 r_2 [p^2, r^{-1}] \\
& - \mu k\, r_1 [r^{-1}, p_2](\vec{r}\cdot\vec{p}) \\
& - \mu k\, r_1 p_2 [r^{-1}, (\vec{r}\cdot\vec{p})] \\
& - \mu k\, p_2 [r_1, (\vec{r}\cdot\vec{p})] r^{-1} \\
& + \mu k\, r_1 r_2 [r^{-1}, p^2] \\
& + \mu k\, r_2 [r_1, p^2] r^{-1} \Big\}
\end{aligned}$$

$$\begin{aligned}
= \mu^{-2}\Big\{ & p_1 (i\hbar p_2)(\vec{r}\cdot\vec{p}) \\
& + p_2 (-i\hbar p_1)(\vec{r}\cdot\vec{p}) \\
& - p_1 (-i\hbar r_2) p^2 \\
& - p_1 r_2 (2i\hbar p^2) \\
& - \mu k\, p_1 (-i\hbar r_2) r^{-1} \\
& - \mu k\, p_1 r_2 (i\hbar r^{-1}) \\
& - \mu k\, r_2 (i\hbar r_1 r^{-3})(\vec{r}\cdot\vec{p}) \\
& - r_1 p_2 (-2i\hbar p^2) \\
& - p_2 (i\hbar r_1) p^2 \\
& + r_1 (-2i\hbar p_2) p^2 \\
& + r_2 (2i\hbar p_1) p^2 \\
& + \mu k\, r_1 (-2i\hbar p_2) r^{-1} \\
& + \mu k\, r_1 r_2 [p^2, r^{-1}] \\
& - \mu k\, r_1 (-i\hbar r_2 r^{-3})(\vec{r}\cdot\vec{p}) \\
& - \mu k\, r_1 p_2 (-i\hbar r^{-1}) \\
& - \mu k\, p_2 (i\hbar r_1) r^{-1} \\
& - \mu k\, r_1 r_2 [p^2, r^{-1}] \\
& + \mu k\, r_2 (2i\hbar p_1) r^{-1} \Big\},
\end{aligned}$$

$$\therefore\ [A_1, A_2] = i\hbar\mu^{-2}\left\{ r_2 p_1 p^2 - r_1 p_2 p^2 - 2\mu k\, r_1 p_2 r^{-1} + 2\mu k\, r_2 p_1 r^{-1} \right\},$$

$$\therefore\ [A_1, A_2] = i\hbar\mu^{-2}\left\{ - L_3 p^2 - 2\mu k\, L_3 r^{-1} \right\},$$

$$\therefore\ [A_1, A_2] = i\hbar\left(\frac{-2}{\mu}\right)\left\{ L_3 \frac{p^2}{2\mu} + L_3 \frac{k}{r} \right\},$$

$$\therefore\ [A_1, A_2] = i\hbar\, L_3\left(-\frac{2H}{\mu}\right);$$

and, from eq. (9.17), it then follows that

$$[K_1, K_2] = i\hbar\, L_3\ ,$$

and, from the isotropy of the problem,

$$[K_i, K_j] = i\hbar\, \varepsilon_{ijk} L_k\,.$$

(v). To show that $H = -\dfrac{\mu k^2}{2}\dfrac{1}{K^2 + L^2 + \hbar^2}$

Consider

$$\begin{aligned}
A_1^2 = \mu^{-2}\{\ & p_1(\vec r\cdot\vec p)p_1(\vec r\cdot\vec p) \\
& - p_1(\vec r\cdot\vec p)\, r_1 p^2 \\
& - \mu k\, p_1(\vec r\cdot\vec p)\, r_1 r^{-1} \\
& - r_1 p^2 p_1(\vec r\cdot\vec p) \\
& + r_1 p^2 r_1 p^2 \\
& + \mu k\, r_1 p^2 r_1 r^{-1} \\
& - \mu k\, r_1 r^{-1} p_1(\vec r\cdot\vec p) \\
& + \mu k\, r_1 r^{-1} r_1 p^2 \\
& + \mu^2 k^2 r_1^2 r^{-2}\ \}
\end{aligned}
\qquad
\begin{aligned}
= \mu^{-2}\{\ & p_1\{p_1(\vec r\cdot\vec p) + i\hbar p_1\}(\vec r\cdot\vec p) \\
& - p_1\{r_1(\vec r\cdot\vec p) - i\hbar r_1\}p^2 \\
& - \mu k\, p_1\{r_1(\vec r\cdot\vec p) - i\hbar r_1\}r^{-1} \\
& - r_1 p^2 p_1(\vec r\cdot\vec p) \\
& + r_1\{r_1 p^2 - 2i\hbar p_1\}p^2 \\
& + \mu k\, r_1\{r_1 p^2 - 2i\hbar p_1\}r^{-1} \\
& - \mu k\, r_1 r^{-1} p_1(\vec r\cdot\vec p) \\
& + \mu k\, r_1 r^{-1} r_1 p^2 \\
& + \mu k^2 r_1^2 r^{-2}\ \}
\end{aligned}$$

Similar expressions follow for A_2^2 and A_3^2, and then from $A^2 = A_1^2 + A_2^2 + A_3^2$:

[cancellation]

$$
\begin{aligned}
A^2 = \mu^{-2}\Big\{ & p^2(\vec{r}\cdot\vec{p})^2 \\
& + i\hbar\, p^2(\vec{r}\cdot\vec{p}) \\
& - (\vec{p}\cdot\vec{r})(\vec{r}\cdot\vec{p})\,p^2 \\
& + i\hbar(\vec{p}\cdot\vec{r})\,p^2 \\
& - \mu k(\vec{p}\cdot\vec{r})(\vec{r}\cdot\vec{p})\,r^{-1} \\
& + i\hbar\mu k(\vec{p}\cdot\vec{r})\,r^{-1} \\
& - (\vec{r}\cdot\vec{p})\,p^2(\vec{r}\cdot\vec{p}) \\
& + r^2p^4 \\
& - 2i\hbar(\vec{r}\cdot\vec{p})\,p^2 \\
& + \mu k\, r^2p^2r^{-1} \\
& - 2i\hbar\mu k(\vec{r}\cdot\vec{p})\,r^{-1} \\
& - \mu k\, r^{-1}(\vec{r}\cdot\vec{p})^2 \\
& + \mu k\, r^{-1}r^2p^2 \\
& + \mu^2k^2 \Big\}
\end{aligned}
\qquad
\begin{aligned}
= \mu^{-2}\Big\{ & p^2(\vec{r}\cdot\vec{p})^2 \\
& + i\hbar\, p^2(\vec{r}\cdot\vec{p}) \\
& - \{(\vec{r}\cdot\vec{p}) - 3i\hbar\}(\vec{r}\cdot\vec{p})\,p^2 \\
& + i\hbar\{(\vec{r}\cdot\vec{p}) - 3i\hbar\}\,p^2 \\
& - \mu k\{(\vec{r}\cdot\vec{p}) - 3i\hbar\}(\vec{r}\cdot\vec{p})\,r^{-1} \\
& + i\hbar\mu k\{(\vec{r}\cdot\vec{p}) - 3i\hbar\}\,r^{-1} \\
& - \{p^2(\vec{r}\cdot\vec{p}) + 2i\hbar p^2\}(\vec{r}\cdot\vec{p}) \\
& + r^2p^4 \\
& - 2i\hbar(\vec{r}\cdot\vec{p})\,p^2 \\
& + \mu k\, r^2p^2r^{-1} \\
& - 2i\hbar\mu k(\vec{r}\cdot\vec{p})\,r^{-1} \\
& - \mu k\, r^{-1}(\vec{r}\cdot\vec{p})^2 \\
& + \mu k\, r^{-1}r^2p^2 \\
& + \mu^2k^2 \Big\}
\end{aligned}
$$

Then, identifying factors:

$$r^2p^2 - (\vec{r}\cdot\vec{p})^2 + i\hbar(\vec{r}\cdot\vec{p}) = L^2;$$

$$
\begin{aligned}
\therefore A^2 = \mu^{-2}\Big\{ & \mu k r^{-1}\{r^2p^2 - (\vec{r}\cdot\vec{p})^2 + i\hbar(\vec{r}\cdot\vec{p})\} && - i\hbar\mu k\, r^{-1}(\vec{r}\cdot\vec{p}) \\
& + \mu k\{r^2p^2 - (\vec{r}\cdot\vec{p})^2 + i\hbar(\vec{r}\cdot\vec{p})\}\,r^{-1} && + i\hbar\mu k(\vec{r}\cdot\vec{p})\,r^{-1} \\
& + \{r^2p^2 - (\vec{r}\cdot\vec{p})^2 + i\hbar(\vec{r}\cdot\vec{p})\}\,p^2 && + i\hbar(\vec{r}\cdot\vec{p})\,p^2 \\
& + \mu^2k^2 + 3\hbar^2p^2 + 3\mu k\hbar^2 r^{-1} && - i\hbar\, p^2(\vec{r}\cdot\vec{p}) \Big\}
\end{aligned}
$$

$$\therefore A^2 = \mu^{-2}\Big\{\mu k r^{-1} L^2 - i\hbar\mu k\cancel{\{(\vec{r}\cdot\vec{p})r^{-1} - i\hbar r^{-1}\}}$$

$$+\mu k L^2 r^{-1} + \cancel{i\hbar\mu k(\vec{r}\cdot\vec{p})r^{-1}}$$

$$+ L^2 p^2 \quad + \cancel{i\hbar(\vec{r}\cdot\vec{p})p^2}$$

$$+\mu^2 k^2 + 3\hbar^2 p^2 + 3\mu k\hbar^2 r^{-1} - i\hbar\cancel{\{(\vec{r}\cdot\vec{p})p^2 - 2i\hbar p^2\}}\Big\}.$$

$$\therefore A^2 = \mu^{-2}\Big\{2\mu\frac{k}{r}L^2 + L^2 p^2 + \mu^2 k^2 + \hbar^2 p^2 + 2\mu k\hbar^2 r^{-1}\Big\},$$

where $[L^2, r^{-1}] = 0$ has been used.

$$\therefore A^2 = \frac{2}{\mu}\Big\{L^2 H + \frac{\mu k^2}{2} + \hbar^2 H\Big\},$$

$$\therefore \frac{-\mu}{2H}A^2 = -L^2 - \frac{\mu k^2}{2H} - \hbar^2 = K^2,$$

$$\therefore \frac{-\mu k^2}{2H} = K^2 + L^2 + \hbar^2,$$

$$\therefore H = \frac{-\mu k^2}{2}\frac{1}{K^2 + L^2 + \hbar^2}.$$

The six operators $\{L_1, L_2, L_3, K_1, K_2, K_3\}$ or $\{L_x, L_y, L_z, K_x, K_y, K_z\}$ form a closed set under commutation, i.e. they form a Lie algebra. Furthermore, the Hamiltonian for the quantum mechanical Kepler problem can be expressed in terms of these operators.

These operators, for $E < 0$ ($k < 0$)* generate the Lie algebra $SO(4)$.

* For $k = 0$ or $k > 0$, the definition of $\vec{K}$ does not lead to an $SO(4)$ algebraic structure. Thus, the use of $SO(4)$ to discuss solutions to the quantum Kepler problem is valid only for bound states.

Thus, we can adopt the algebraic properties of SO(4) to elucidate the structure of the quantum Kepler problem.

The SO(4) Lie algebra of interest here can be defined by:

$$[L_i, L_j] = i\hbar\, \varepsilon_{ijk} L_k , \qquad 9.22$$

$$[K_i, K_j] = i\hbar\, \varepsilon_{ijk} L_k , \qquad 9.23$$

$$[L_i, K_j] = i\hbar\, \varepsilon_{ijk} K_k . \qquad 9.24$$

Further, for

$$L^2 = L_1^2 + L_2^2 + L_3^2 , \qquad 9.25$$

$$K^2 = K_1^2 + K_2^2 + K_3^2 , \qquad 9.26$$

it follows in a manner identical to the development in Section 5. that

$$[L^2, L_i] = 0, \qquad i = 1, 2, 3. \qquad 9.27$$

Further,

$$[K^2, L_i] = 0, \qquad i = 1, 2, 3, \qquad 9.28$$

$$[L^2 + K^2, K_i] = 0, \qquad i = 1, 2, 3, \qquad 9.29$$

and

$$[L^2, K^2] = 0. \qquad 9.30$$

The operators $\{L_1, L_2, L_3\}$ manifestly define an SO(3) subalgebra. (This corresponds to the subgroup of rotations.) However, the operators $\{K_1, K_2, K_3\}$ are "entangled" with these SO(3) operators.

A "disentanglement" of the SO(4) operators can be effected by defining

$$\vec{M} = \tfrac{1}{2}(\vec{L}+\vec{K}), \tag{9.31}$$

$$\vec{N} = \tfrac{1}{2}(\vec{L}-\vec{K}); \tag{9.32}$$

whence

$$[M_i, M_j] = i\hbar\, \varepsilon_{ijk} M_k \tag{9.33}$$

$$[N_i, N_j] = i\hbar\, \varepsilon_{ijk} N_k \tag{9.34}$$

$$[M_i, N_j] = 0, \quad \forall\, i,j \in 1,2,3 \tag{9.35}$$

$$[M^2, M_i] = 0, \quad i = 1,2,3 \tag{9.36}$$

$$[M^2, N_i] = 0, \quad i = 1,2,3 \tag{9.37}$$

$$[N^2, M_i] = 0, \quad i = 1,2,3 \tag{9.38}$$

$$[N^2, N_i] = 0, \quad i = 1,2,3 \tag{9.39}$$

$$[M^2, N^2] = 0. \tag{9.40}$$

Thus, the operators $\{M_1, M_2, M_3\}$ and $\{N_1, N_2, N_3\}$ form two subalgebras: They are each $SU(2)$ algebras. We indicate this by

$$SO(4) = SU(2) \times SU(2), \tag{9.41}$$

i.e. SO(4) can be reduced to the product of two SU(2) subalgebras. One can proceed to elucidate the quantum structure by adopting the method of raising and lowering operators which provide such an elegant solution to SU(2).

Defining operators

$$M_\pm = M_1 \pm i M_2 \quad , \quad M_0 = M_3 \; , \tag{9.42}$$

$$N_\pm = N_1 \pm i N_2 \quad , \quad N_0 = N_3 \; ; \tag{9.43}$$

then

$$[M_0, M_\pm] = \pm\hbar M_\pm \quad , \quad [M_+, M_-] = 2\hbar M_0 \; , \tag{9.44}$$

$$[N_0, N_\pm] = \pm\hbar N_\pm \quad , \quad [N_+, N_-] = 2\hbar N_0 \; , \tag{9.45}$$

$$M^2 |j_m m_m\rangle = j_m (j_m + 1)\hbar^2 |j_m m_m\rangle \; , \tag{9.46}$$

$$M_0 |j_m m_m\rangle = m_m \hbar |j_m m_m\rangle , \quad m_m = j_m, j_m - 1, \ldots, -j_m \; , \tag{9.47}$$

$$N^2 |j_n m_n\rangle = j_n (j_n + 1)\hbar^2 |j_n m_n\rangle \; , \tag{9.48}$$

$$N_0 |j_n m_n\rangle = m_n \hbar |j_n m_n\rangle , \quad m_n = j_n, j_n - 1, \ldots, -j_n \; , \tag{9.49}$$

$$M_\pm |j_m m_m\rangle = \sqrt{(j_m \mp m_m)(j_m \pm m_m + 1)}\,\hbar\, |j_m m_m \pm 1\rangle \; , \tag{9.50}$$

$$N_\pm |j_n m_n\rangle = \sqrt{(j_n \mp m_n)(j_n \pm m_n + 1)}\,\hbar\, |j_n m_n \pm 1\rangle . \tag{9.51}$$

The Hamiltonian can now be written

$$H = \frac{-\mu k^2}{2} \frac{1}{2M^2 + 2N^2 + \hbar^2} \; ; \qquad 9.52$$

and immediately it follows that the energy eigenvectors are $|j_m m_m j_n m_n\rangle$, and the energy eigenvalues are

$$E(j_m j_n) = \frac{-\mu k^2}{4\hbar^2} \frac{1}{\{j_m(j_m+1) + j_n(j_n+1) + \frac{1}{2}\}} \; . \qquad 9.53$$

Naively, we could suppose that

$$j_m = 0, \tfrac{1}{2}, 1, \tfrac{3}{2}, \ldots \quad , \quad j_n = 0, \tfrac{1}{2}, 1, \tfrac{3}{2}, \ldots \qquad 9.54$$

However, j_m and j_n are not independent. This has its origin in the relations (cf. eq. (9.13)):

$$\vec{L} \cdot \vec{A} = \vec{A} \cdot \vec{L} = 0 ,$$

whence, from eqs. (9.31, 32),

$$(\vec{M} + \vec{N}) \cdot (\vec{M} - \vec{N}) = (\vec{M} - \vec{N}) \cdot (\vec{M} + \vec{N}) = 0 . \qquad 9.55$$

$$\therefore M^2 - \vec{M}\cdot\vec{N} + \vec{N}\cdot\vec{M} - N^2 = M^2 + \vec{M}\cdot\vec{N} - \vec{N}\cdot\vec{M} - N^2 = 0 . \qquad 9.56$$

It then follows that

$$\vec{M} \cdot \vec{N} = \vec{N} \cdot \vec{M} \qquad 9.57$$

and

$$M^2 = N^2 . \qquad 9.58$$

Thus, we require

$$j_m = j_n = 0, \tfrac{1}{2}, 1, \tfrac{3}{2}, \ldots \equiv \nu \qquad 9.59$$

and so

$$E_\nu = \frac{-\mu k^2}{2\hbar^2} \frac{1}{(2\nu+1)^2} \; , \quad \nu = 0, \tfrac{1}{2}, 1, \tfrac{3}{2}, \ldots \qquad 9.60$$

Thus, for $k^2 = (-e^2/4\pi\epsilon_0)^2$ and $2\nu+1 = n$,

$$E_n = -\frac{R_y}{n^2}, \quad n = 1, 2, 3, \ldots, \qquad 9.61$$

where

$$R_y = \frac{\mu e^4}{8\epsilon_0^2 h^2} = 13.606 \text{ eV}, \qquad 9.62$$

i.e. the Rydberg formula for the hydrogen atom.

The degeneracies of the problem emerge from the eigenvalue spectra of j_m, m_m, j_n, m_n and the relations (cf. eqs. (9.31, 32))

$$M_0 = \tfrac{1}{2}(L_0 + K_0), \qquad 9.63$$

$$N_0 = \tfrac{1}{2}(L_0 - K_0), \qquad 9.64$$

whence it follows that:

$j_m = j_n = 0$, $m_m = m_n = 0$, $m_\ell = 0$, $m_k = 0$,

$j_m = j_n = \tfrac{1}{2}$, $m_m = \pm\tfrac{1}{2}$, $m_n = \pm\tfrac{1}{2}$, $(m_\ell, m_k) = (1,0), (0,1), (0,-1), (-1,0)$

$j_m = j_n = 1$, $m_m = 0, \pm 1$, $m_n = 0, \pm 1$,
$(m_\ell, m_k) = (2,0), (1,1), (0,2), (1,-1), (0,0), (-1,1), (0,-2), (-1,-1), (-2,0)$

and so on; where m_ℓ, m_k are the quantum numbers labelling L_0 and K_0 (recall $[L_0, K_0] = 0$). Thus:

for $j_m = j_n = 0$, $\ell = 0$,

for $j_m = j_n = \tfrac{1}{2}$, $\ell = 0$ or 1,

for $j_m = j_n = 1$, $\quad l = 0, 1,$ or 2,
etc.,

where $m_l = l, l-1, \ldots, -l$ has been used. There is an elegant graphical method of representing the $so(4)$ irreps, $\mathcal{D}^{j_m, j_n}$, shown in Fig. 9.3 (we revert to L_z, K_z, M_z, N_z (= L_0, K_0, M_0, N_0,

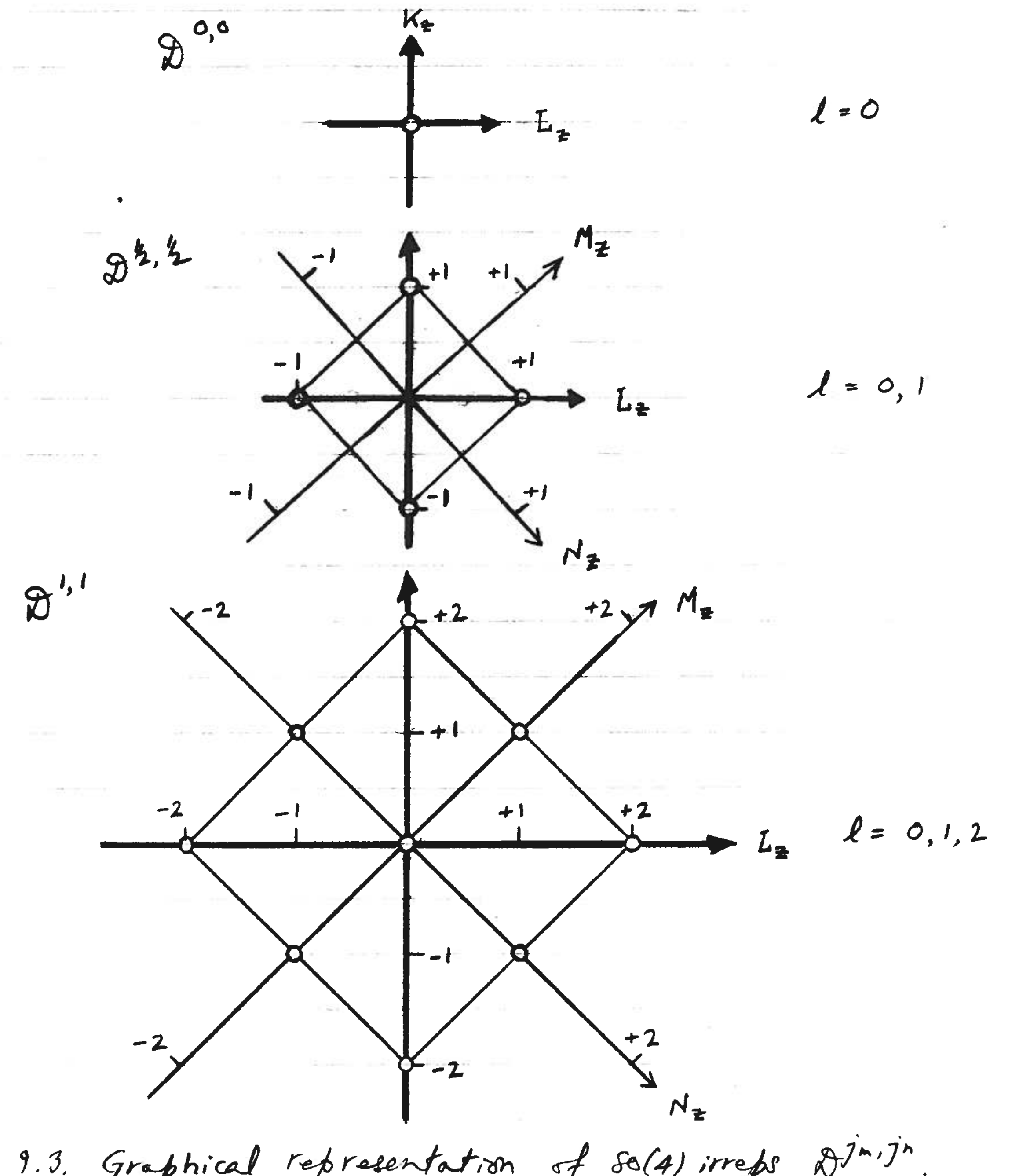

Fig. 9.3. Graphical representation of $so(4)$ irreps $\mathcal{D}^{j_m, j_n}$.

respectively) here). The values of l occurring in each SO(4) irrep (cf. Fig. 9.3) are ascertained from the multiplicities of each L_z eigenvalue. So one obtains the spectrum

$$l = l_{max},\ l_{max}-1, \ldots 1, 0, \qquad 9.65$$

where

$$l_{max} = j_m + j_n = n-1. \qquad 9.66$$

The diagrams for $\mathcal{D}^{j_m, j_n}$ are called <u>weight diagrams</u>. (It should be noted that the irreps of SO(4) are labelled by (j_m, j_n) where j_m and j_n can take any combination of the values $j_m = 0, \frac{1}{2}, 1, \frac{3}{2}, \ldots, j_n = 0, \frac{1}{2}, 1, \frac{3}{2}, \ldots$: However, this full range of possibilities is not realized in the quantum Kepler problem because of the constraint $j_m = j_n$ which results from $\vec{A}\cdot\vec{L} = \vec{L}\cdot\vec{A} = 0$, i.e. $\vec{A}$ and $\vec{L}$ are perpendicular to each other.)

The weight diagrams of SO(4) define a two-dimensional space called <u>weight space</u>. (The weight space for SO(3) is one dimensional.) The action of the raising and lowering operators in weight space can be depicted using <u>root diagrams</u>. The root diagram for $M_\pm$, $N_\pm$ for SO(4) is shown in Fig. 9.4. The $M_\pm, N_\pm$ raising and lowering operators shift M_z and N_z according to:

$$[M_z, M_\pm] = \pm\hbar\, M_\pm \quad , \quad [N_z, N_\pm] = \pm\hbar\, N_\pm \ , \qquad 9.67$$

$$[M_z, N_\pm] = 0 \quad , \quad [N_z, M_\pm] = 0\ ; \qquad 9.68$$

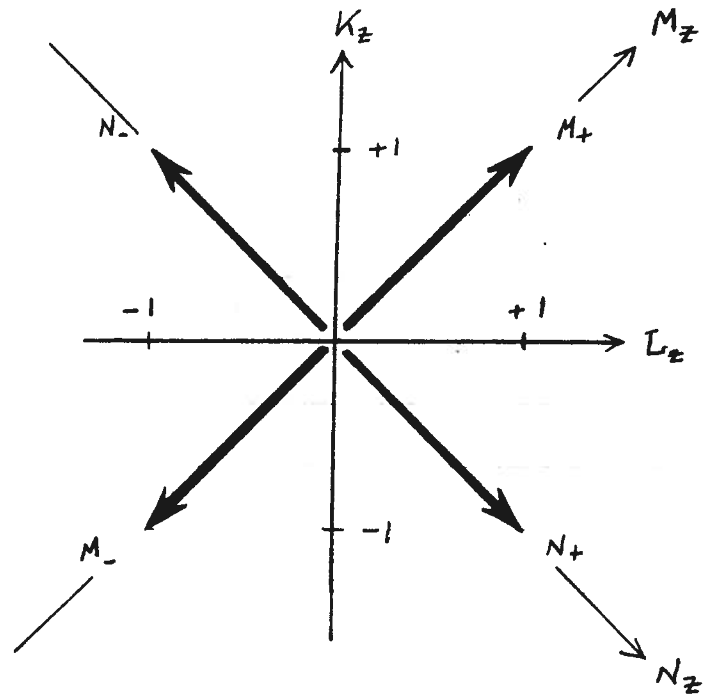

Fig. 9.4. The SO(4) root diagram for the $M_\pm$, $N_\pm$ raising and lowering or shift operators.

and they shift I_z and K_z according to:

$$[I_z, M_\pm] = \pm\hbar M_\pm, \quad [K_z, M_\pm] = \pm\hbar M_\pm, \qquad 9.69$$

$$[I_z, N_\pm] = \pm\hbar N_\pm, \quad [K_z, N_\pm] = \mp\hbar N_\pm. \qquad 9.70$$

These actions are readily discerned in Fig. 9.4. The so(4) Lie algebra is said to have <u>rank two</u> because its weight space is two dimensional. Technically, this has its origin in the two mutually commuting so(4) generators: I_z and K_z.

A subtle point that arises is the connection between the weight diagrams and the quantum number l. The states depicted in the weight diagrams are labelled by either L_z, K_z quantum numbers, i.e. m_l, m_K, or by M_z, N_z quantum numbers, i.e. m_m, m_n. In each SO(4) irrep (Fig. 9.3) the values of l occurring are ascertained from the multiplicities of each m_l value ($m_l = 0, 1, 2, \ldots$): this is called the <u>m scheme</u>. However, the states in the weight diagrams do not necessarily have well-defined l values! This is because L^2 and K_z do not commute and, thus, l and m_K are not compatible constants of the motion. The states in the weight diagram have well-defined energy, m_l, m_K, m_m, m_n, j_m, and j_n. States of good l can be constructed from the weight diagram by noting the relationships $\vec{L} = \vec{M} + \vec{N}$, $L_z = M_z + N_z$ (cf. eqs. (9.31, 32)). Thus, eigenstates of l are obtained by coupling j_m, j_n eigenstates:

$$|l\, m_l\rangle = \sum_{m_m} |j_m m_m j_n m_n\rangle \langle j_m m_m j_n m_n | l\, m_l\rangle ; \qquad 9.71$$

where $\langle j_m m_m j_n m_n | l\, m_l\rangle$ is a Clebsch-Gordan coefficient; and in a given irrep j_m and j_n are fixed, $m_m + m_n = m_l$, and $|j_m - j_n| \leq l \leq j_m + j_n$ implies $0 \leq l \leq 2\nu$ (cf. eqs (9.65, 66)). Thus, in the separation $SO(4) = SU_m(2) \times SU_n(2)$, where the SU(2)'s are labelled by j_m, j_n: neither of these SU(2)'s is the one labelled by l, i.e neither of these SU(2)'s is the angular momentum $SU(2) \approx SO(3) \equiv SO_l(3)$. One distinguishes between these two possibilities by writing:

$$SO(4) = SU_m(2) \times SU_n(2), \qquad 9.72$$

$$SO(4) \supset SO_\ell(3), \qquad 9.73$$

where "$\supset$" means "has the subalgebra".

The three different subalgebras, $SU_m(2)$, $SU_n(2)$, and $SO_\ell(3)$ in eqs. (9.72, 73) can be distinguished by their generators:

$$SU_m(2): \quad M_x = \frac{L_x + K_x}{2}, \quad M_y = \frac{L_y + K_y}{2}, \quad M_z = \frac{L_z + K_z}{2}, \qquad 9.74$$

$$SU_n(2): \quad N_x = \frac{L_x - K_x}{2}, \quad N_y = \frac{L_y - K_y}{2}, \quad N_z = \frac{L_z - K_z}{2}, \qquad 9.75$$

$$SO_\ell(3): \quad L_x, L_y, L_z. \qquad 9.76$$

The three operators $\{K_x, K_y, K_z\}$ do not close under commutation (cf. eq. (9.18)) and so they do not form a subalgebra of $SO(4)$. The $SU_m(2)$, $SU_n(2)$, and $SO_\ell(3)$ subalgebras of $SO(4)$ illustrate some of the ways in which different types of subalgebraic structure can arise for a given algebra. Only the $SO_\ell(3)$ subalgebra is associated with physically observable quantities. The $SU_m(2)$ and $SU_n(2)$ subalgebras are introduced purely to solve the problem: they provide the quantum numbers -- j_m, j_n -- that uniquely label the $SO(4)$ irreps. The $SO_\ell(3)$ quantum number ℓ does not offer a way of labelling $SO(4)$ irreps. (It often happens that the physically interesting subalgebras are not able to provide useful labels for irreps and, conversely, that irrep labels are not physically interesting.)

Appendix: Commutator Bracket Relations for Central Force Problems

I. For vector operators $\vec{A}$, $\vec{B}$, and $\vec{C}$:

$$(\vec{A}\times\vec{B})\times\vec{C} = (\vec{A}\cdot\vec{C})\vec{B} - \vec{A}(\vec{B}\cdot\vec{C})$$
$$+ \left(A_1[B_1,C_1] + A_2[B_1,C_2] + A_3[B_1,C_3]\right)\hat{i}$$
$$+ \left(A_1[B_2,C_1] + A_2[B_2,C_2] + A_3[B_2,C_3]\right)\hat{j}$$
$$+ \left(A_1[B_3,C_1] + A_2[B_3,C_2] + A_3[B_3,C_3]\right)\hat{k}. \qquad 9A.1$$

Proof: from the left-hand side,

$$\vec{A}\times\vec{B} = \begin{vmatrix} \hat{i} & \hat{j} & \hat{k} \\ A_1 & A_2 & A_3 \\ B_1 & B_2 & B_3 \end{vmatrix} = (A_2B_3 - A_3B_2)\hat{i} + (A_3B_1 - A_1B_3)\hat{j} + (A_1B_2 - A_2B_1)\hat{k},$$

(note the order of the $A_i B_j$);

$$\therefore (\vec{A}\times\vec{B})\times\vec{C} = \begin{vmatrix} \hat{i} & \hat{j} & \hat{k} \\ A_2B_3 - A_3B_2 & A_3B_1 - A_1B_3 & A_1B_2 - A_2B_1 \\ C_1 & C_2 & C_3 \end{vmatrix},$$

$$\therefore (\vec{A}\times\vec{B})\times\vec{C} = (A_3B_1C_3 - A_1B_3C_3 - A_1B_2C_2 + A_2B_1C_2)\hat{i}$$
$$+ (A_1B_2C_1 - A_2B_1C_1 - A_2B_3C_3 + A_3B_2C_3)\hat{j}$$
$$+ (A_2B_3C_2 - A_3B_2C_2 - A_3B_1C_1 + A_1B_3C_1)\hat{k}.$$

From the right-hand side, for the $\hat{i}$ term

$$\text{"}\hat{i}\text{ term"} = \cancel{A_1C_1B_1} + \cancel{A_2C_2B_1} + \cancel{A_3C_3B_1} - \cancel{A_1B_1C_1} - A_1B_2C_2 - A_1B_3C_3$$
$$+ \cancel{A_1B_1C_1} - \cancel{A_1C_1B_1} + A_2B_1C_2 - \cancel{A_2C_2B_1} + A_3B_1C_3 - \cancel{A_3C_3B_1}$$

$$= A_3B_1C_3 - A_1B_3C_3 - A_1B_2C_2 + A_2B_1C_2$$

Similarly for the $\hat{j}$ and $\hat{k}$ terms, whence eq. (9A.1) follows.

Also

$$\vec{A} \times (\vec{B} \times \vec{C}) = (\vec{A} \cdot \vec{C})\vec{B} - (\vec{A} \cdot \vec{B})\vec{C}$$
$$+ (A_1[B_1, C_1] + A_2[B_1, C_2] + A_3[B_1, C_3])\hat{i}$$
$$+ (A_1[B_2, C_1] + A_2[B_2, C_2] + A_3[B_2, C_3])\hat{j}$$
$$+ (A_1[B_3, C_1] + A_2[B_3, C_2] + A_3[B_3, C_3])\hat{k}, \quad 9A.2$$

$$\therefore \vec{A} \times (\vec{B} \times \vec{C}) = (\vec{A} \times \vec{B}) \times \vec{C} + \vec{A}(\vec{B} \cdot \vec{C}) - (\vec{A} \cdot \vec{B})\vec{C}. \quad 9A.3$$

II. From

$$[r_i, p_j] = i\hbar\, \delta_{ij} \quad 9A.4$$

and

$$[p_j, f(r_1, r_2, r_3)] = -i\hbar \frac{\partial f}{\partial r_j} \quad 9A.5$$

$$[r_j, f(p_1, p_2, p_3)] = i\hbar \frac{\partial f}{\partial p_j} \quad 9A.6$$

a). $\vec{r} \cdot \vec{p} = r_1 p_1 + r_2 p_2 + r_3 p_3$,

$\therefore \vec{r} \cdot \vec{p} = p_1 r_1 + p_2 r_2 + p_3 r_3 + 3i\hbar$,

$$\therefore \vec{r} \cdot \vec{p} = \vec{p} \cdot \vec{r} + 3i\hbar. \quad 9A.7$$

b). $[r_1, p^2] = i\hbar \dfrac{\partial}{\partial p_1}(p_1^2 + p_2^2 + p_3^2)$,

$$\therefore [r_1, p^2] = 2i\hbar\, p_1 \quad 9A.8$$

c). $[p_1, r^{-1}] = -i\hbar \dfrac{\partial}{\partial r_1}\left\{(r_1^2 + r_2^2 + r_3^2)^{-1/2}\right\}$,

$\therefore [p_1, r^{-1}] = -i\hbar \left(\dfrac{-1}{2}\right)(r_1^2 + r_2^2 + r_3^2)^{-3/2}\, 2r_1$,

$\therefore [p_1, r^{-1}] = i\hbar\, r_1\, r^{-3}$. 9A.9

d). $[p^2, r^{-1}] = [(p_1^2 + p_2^2 + p_3^2), r^{-1}]$,

$\therefore [p^2, r^{-1}] = p_1[p_1, r^{-1}] + [p_1, r^{-1}]p_1$ etc.,

$\therefore [p^2, r^{-1}] = i\hbar(p_1 r_1 r^{-3} + r_1 r^{-3} p_1)$ etc.,

$\therefore [p^2, r^{-1}] = i\hbar\{(\vec{p}\cdot\vec{r})r^{-3} + r^{-3}(\vec{r}\cdot\vec{p})\}$. 9A.10

e). $[r_1, (\vec{r}\cdot\vec{p})] = [r_1, (r_1 p_1 + r_2 p_2 + r_3 p_3)]$,

$\therefore [r_1, (\vec{r}\cdot\vec{p})] = r_1 [r_1, p_1]$,

$\therefore [r_1, (\vec{r}\cdot\vec{p})] = i\hbar r_1$. 9A.11

f). $[p_1, (\vec{r}\cdot\vec{p})] = [p_1, (r_1 p_1 + r_2 p_2 + r_3 p_3)]$,

$\therefore [p_1, (\vec{r}\cdot\vec{p})] = -i\hbar p_1$. 9A.12

g). $[(\vec{r}\cdot\vec{p}), r^{-1}] = [(r_1 p_1 + r_2 p_2 + r_3 p_3), r^{-1}]$,

$\therefore [(\vec{r}\cdot\vec{p}), r^{-1}] = r_1 [p_1, r^{-1}] + r_2 [p_2, r^{-1}] + r_3 [p_3, r^{-1}]$,

$$\therefore [(\vec{r}\cdot\vec{p}), r^{-1}] = r_1(-i\hbar r_1 r^{-3}) + r_2(i\hbar r_2 r^{-3}) + r_3(i\hbar r_3 r^{-3}),$$

$$\therefore [(\vec{r}\cdot\vec{p}), r^{-1}] = i\hbar r^{-1}. \qquad 9A.13$$

h). $[(\vec{r}\cdot\vec{p}), p^2] = [(r_1p_1 + r_2p_2 + r_3p_3), p^2],$

$$\therefore [(\vec{r}\cdot\vec{p}), p^2] = [r_1, p^2]p_1 + [r_2, p^2]p_2 + [r_3, p^2]p_3,$$

$$\therefore [(\vec{r}\cdot\vec{p}), p^2] = 2i\hbar p^2. \qquad 9A.14$$

i). $[(\vec{r}\cdot\vec{p}), r^{-3}] = [(r_1p_1 + r_2p_2 + r_3p_3), (r_1^2 + r_2^2 + r_3^2)^{-3/2}],$

$$\therefore [(\vec{r}\cdot\vec{p}), r^{-3}] = r_1(-i\hbar)\left(\frac{-3}{2}\right)(r_1^2+r_2^2+r_3^2)^{-5/2}\, 2r_1 \quad \text{etc.},$$

$$\therefore [(\vec{r}\cdot\vec{p}), r^{-3}] = 3i\hbar\,(r_1^2+r_2^2+r_3^2)(r_1^2+r_2^2+r_3^2)^{-5/2},$$

$$\therefore [(\vec{r}\cdot\vec{p}), r^{-3}] = 3i\hbar r^{-3}. \qquad 9A.15$$

These results and their generalizations are presented in Table 9A.1.

Table 9A.1. Operator relations and commutator bracket relations for central force problems.	
$[p_j, f(r_1, r_2, r_3, p_1, p_2, p_3)] = -i\hbar \dfrac{\partial f}{\partial r_j}.$	9A.16
$[r_j, f(r_1, r_2, r_3, p_1, p_2, p_3)] = i\hbar \dfrac{\partial f}{\partial p_j}.$	9A.17

(cont.)

$$\vec{r}\cdot\vec{p} = \vec{p}\cdot\vec{r} + 3i\hbar. \qquad 9A.18$$

$$[r_1, p^2] = 2i\hbar p_1, \quad [r_2, p^2] = 2i\hbar p_2, \quad [r_3, p^2] = 2i\hbar p_3. \qquad 9A.19$$

$$[\vec{r}, p^2] = 2i\hbar\vec{p}. \qquad 9A.20$$

$$[p_1, r^{-1}] = i\hbar r_1 r^{-3}, \quad [p_2, r^{-1}] = i\hbar r_2 r^{-3}, \quad [p_3, r^{-1}] = i\hbar r_3 r^{-3}. \qquad 9A.21$$

$$[\vec{p}, r^{-1}] = i\hbar\vec{r}\, r^{-3}. \qquad 9A.22$$

$$[p^2, r^{-1}] = i\hbar\{(\vec{p}\cdot\vec{r})r^{-3} + r^{-3}(\vec{r}\cdot\vec{p})\}. \qquad 9A.23$$

$$[r_1, (\vec{r}\cdot\vec{p})] = i\hbar r_1, \quad [r_2, (\vec{r}\cdot\vec{p})] = i\hbar r_2, \quad [r_3, (\vec{r}\cdot\vec{p})] = i\hbar r_3. \qquad 9A.24$$

$$[\vec{r}, (\vec{r}\cdot\vec{p})] = i\hbar\vec{r}. \qquad 9A.25$$

$$[p_1, (\vec{r}\cdot\vec{p})] = -i\hbar p_1, \quad [p_2, (\vec{r}\cdot\vec{p})] = -i\hbar p_2, \quad [p_3, (\vec{r}\cdot\vec{p})] = -i\hbar p_3. \qquad 9A.26$$

$$[\vec{p}, (\vec{r}\cdot\vec{p})] = -i\hbar\vec{p}. \qquad 9A.27$$

$$[(\vec{r}\cdot\vec{p}), r^{-1}] = i\hbar r^{-1}. \qquad 9A.28$$

$$[(\vec{r}\cdot\vec{p}), p^2] = 2i\hbar p^2. \qquad 9A.29$$

$$[(\vec{r}\cdot\vec{p}), r^{-3}] = 3i\hbar r^{-3}. \qquad 9A.30$$

III. For the Lenz vector $\vec{A}$:

$$\vec{A} = \frac{1}{2\mu}\left\{\vec{L}\times\vec{p} - \vec{p}\times\vec{L}\right\} - k\frac{\vec{r}}{r} = \frac{1}{\mu}\left\{\vec{p}(\vec{r}\cdot\vec{p}) - \vec{r}p^2 - \mu k\frac{\vec{r}}{r}\right\}. \quad 9A.31$$

Proof: from the left-hand side of eq. (9A.31), using eqs. (9A.1, 2),

$$\frac{1}{2\mu}\left\{\vec{L}\times\vec{p} - \vec{p}\times\vec{L}\right\} = \frac{1}{2\mu}\left\{(\vec{r}\times\vec{p})\times\vec{p} - \vec{p}\times(\vec{r}\times\vec{p})\right\}$$

$$= \frac{1}{2\mu}\left\{(\vec{r}\cdot\vec{p})\vec{p} - \vec{r}p^2 - p^2\vec{r} + (\vec{p}\cdot\vec{r})\vec{p} - p_1[r_1, p_1]\hat{i} - p_2[r_2, p_2]\hat{j} - p_3[r_3, p_3]\hat{k}\right\}$$

$$= \frac{1}{2\mu}\left\{(\vec{r}\cdot\vec{p})\vec{p} - \vec{r}p^2 - p^2\vec{r} + (\vec{p}\cdot\vec{r})\vec{p} - i\hbar\vec{p}\right\}.$$

Then, using eq. (9A.18 and 20)

$$\frac{1}{2\mu}\left\{\vec{L}\times\vec{p} - \vec{p}\times\vec{L}\right\} = \frac{1}{2\mu}\left\{(\vec{r}\cdot\vec{p})\vec{p} - \vec{r}p^2 - \vec{r}p^2 + \cancel{2i\hbar\vec{p}} + (\vec{r}\cdot\vec{p})\vec{p} - \overset{2}{\cancel{3}}i\hbar - \cancel{i\hbar\vec{p}}\right\},$$

whence from eq. (9A.27)

$$\frac{1}{2\mu}\left\{\vec{L}\times\vec{p} - \vec{p}\times\vec{L}\right\} = \frac{1}{2\mu}\left\{2\vec{p}(\vec{r}\cdot\vec{p}) + \cancel{2i\hbar\vec{p}} - 2\vec{r}p^2 - \cancel{2i\hbar\vec{p}}\right\}.$$

$$\therefore \frac{1}{2\mu}\left\{\vec{L}\times\vec{p} - \vec{p}\times\vec{L}\right\} = \frac{1}{\mu}\left\{\vec{p}(\vec{r}\cdot\vec{p}) - \vec{r}p^2\right\},$$

and, thus, eq. (9A.31) follows.