

Chapter 12

Central Force Problems

The general central force problem in quantum mechanics is solved using a variety of techniques. These are all algebraic: a substantial deviation from the “standard” quantum mechanical treatment of these problems, which are traditionally solved using series solutions of second-order differential equations. The first method uses factorization; the second method uses identification of an $so(2,1)$ algebra as the universal algebraic structure of solvable central-force problems. The methods are used to solve the non-relativistic hydrogen atom, the three-dimensional harmonic oscillator, and the infinite three-dimensional square well system. The connection of the algebra to wave functions is made in Appendix B.

Concepts: centrifugal potential; radial momentum; isospectral Hamiltonians; zero-point energy; spherical Bessel functions; non-compact algebras.

12.1 General features of central force problems

Central force problems in quantum mechanics are a fundamental topic. All of atomic structure and hadronic (baryonic and mesonic) structure and a significant fraction of nuclear structure is based on the general theory of central force problems. Although most atoms are many-electron systems and most nuclei are many-nucleon systems (and all baryons are three-quark systems), the essential problem is that of a single particle moving in a spherically symmetrical potential. (In all these systems, to a first approximation, the many-particle motion is described by an ensemble of independently moving particles.)

A spherically symmetric potential $V(r)$ gives rise to the general Hamiltonian operator.

$$\hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{r}), \quad (12.1)$$

for a quantum mechanical central force problem. The spherical symmetry leads to angular momentum being a conserved quantity or constant of the motion. Thus, l is a good quantum number for central force problems. Formally, this can be expressed as

$$[\hat{H}, \hat{L}^2] = 0. \quad (12.2)$$

The potential $V(r)$ is either a two-body potential (for hydrogen-like or mesonic, i.e., quark-antiquark, systems) or a mean-field potential (for many-electron atomic, nuclear, or baryonic systems). Mean-field potentials are usually prescribed by a suitable model description of the system (e.g., the use of an harmonic oscillator potential or of an infinite square-well potential to describe nuclei.) The mass m is the reduced mass if the potential is two-body and it is an effective mass if a mean-field potential is used.

Since all electrons, all nucleons (protons and neutrons), and all quarks are spin-1/2 particles, all atomic, nuclear, and hadronic systems require the correct quantum mechanical coupling of orbital angular momentum and intrinsic spin. For the present discussion, spin-orbit and spin-spin interactions are not included.

The Hamiltonian for a general central force problem, eq. 12.1, can be expressed in the form

$$H = \frac{p_r^2}{2m} + V(r) + \frac{L^2}{2mr^2}; \quad (12.3)$$

where the (classical mechanical) identity¹

$$L^2 = r^2 p^2 - (\vec{r} \cdot \vec{p})^2 \quad (12.4)$$

has been used, and

$$p_r := \frac{1}{r} \vec{r} \cdot \vec{p}. \quad (12.5)$$

The dynamical quantity p_r is sometimes called the radial momentum. The term $L^2/2mr^2$ is called the centrifugal potential.

The Hamiltonian for a general quantum mechanical central force problem can be expressed in the form

$$\hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{r}) + \frac{\hat{L}^2}{2m\hat{r}^2}, \quad (12.6)$$

where

$$[\hat{r}, \hat{p}_r] = i\hbar, \quad (12.7)$$

and

$$\hat{p}_r := \frac{1}{2} \left\{ \frac{\vec{r}_{\text{op}}}{\hat{r}} \cdot \vec{p}_{\text{op}} + \vec{p}_{\text{op}} \cdot \frac{\vec{r}_{\text{op}}}{\hat{r}} \right\}, \quad (12.8)$$

i.e., eq. 12.8 is symmetrised in \vec{r}_{op} and \vec{p}_{op} . The quantum mechanical versions of eqs. 12.4 and 12.5 are

$$\hat{L}^2 = \hat{r}^2 \hat{p}^2 - (\vec{r}_{\text{op}} \cdot \vec{p}_{\text{op}})(\vec{r}_{\text{op}} \cdot \vec{p}_{\text{op}}) + i\hbar(\vec{r}_{\text{op}} \cdot \vec{p}_{\text{op}}), \quad (12.9)$$

and

$$\hat{p}_r = \frac{1}{\hat{r}} \vec{r}_{\text{op}} \cdot \vec{p}_{\text{op}} - \frac{i\hbar}{\hat{r}}, \quad (12.10)$$

respectively. More details of commutator bracket relations for central force problems are given in Appendix A.

¹This follows from $L^2 = (\vec{r} \times \vec{p}) \cdot (\vec{r} \times \vec{p})$ and the identity $(\vec{A} \times \vec{B}) \cdot (\vec{A} \times \vec{B}) = (\vec{A} \cdot \vec{A})(\vec{B} \cdot \vec{B}) - (\vec{A} \cdot \vec{B})^2$.

Quantum mechanical central force problems are defined by the eigenvalue equations:

$$\hat{H}|\alpha lm\rangle = E_{\alpha l}|\alpha lm\rangle, \quad (12.11)$$

$$\hat{L}^2|\alpha lm\rangle = l(l+1)\hbar^2|\alpha lm\rangle, \quad (12.12)$$

$$\hat{L}_z|\alpha lm\rangle = m\hbar|\alpha lm\rangle, \quad (12.13)$$

where $\{\hat{H}, \hat{L}^2, \hat{L}_z\}$ form a set of mutually commuting operators and α labels the energy eigenvalues. The energy eigenvalues will also depend on l because, from eqs. 12.6 and 12.12,

$$\hat{H} := \hat{H}_l = \frac{\hat{p}_r^2}{2m} + V(\hat{r}) + \frac{l(l+1)\hbar^2}{2m\hat{r}^2}; \quad (12.14)$$

i.e., the total potential $W_l(\hat{r})$,

$$W_l(\hat{r}) := V(\hat{r}) + \frac{l(l+1)\hbar^2}{2m\hat{r}^2}, \quad l = 0, 1, 2, \dots, \quad (12.15)$$

depends on l . (The inclusion of \hat{L}_z in the set of mutually commuting operators can only be made provided \hat{H} does not contain a spin-orbit coupling term, cf. Ex. 11-6. Spin-orbit coupling in central force problems is included after solutions for $E_{\alpha l}$ have been discussed.)

The total potential $W_l(\hat{r})$ provides a useful view of the manner in which a (quantum mechanical) particle moving in a central field is confined as a function of r and l . This is illustrated in Fig. 12.1 for a three-dimensional finite square well, i.e.,

$$V(r) = -V_0, \quad r < R, \quad (12.16)$$

$$V(r) = 0, \quad r \geq R. \quad (12.17)$$

The classification of the Hamiltonian \hat{H} into a family of Hamiltonians $\hat{H}_l, l = 0, 1, 2, \dots$, provides a remarkable simplification for solving the energy eigenvalue problem.

The Hamiltonian for any central force problem can be expressed in the general form, eq. 12.14.

12.2 Central force problems and factorisation algebra

Defining the zero-point energy in the potential $W_l(\hat{r})$ to be E_{1l} , consider:

$$\begin{aligned} \hat{H}_l - E_{1l} &= \frac{1}{2m} \left\{ \hat{p}_r - i \left(f(\hat{r}) + \frac{(l+1)\hbar}{\hat{r}} \right) \right\} \left\{ \hat{p}_r + i \left(f(\hat{r}) + \frac{(l+1)\hbar}{\hat{r}} \right) \right\} \\ &= \frac{\hat{p}_r^2}{2m} + \frac{i}{2m} [\hat{p}_r, f(\hat{r})] - i\hbar f'(\hat{r}) + \frac{i\hbar(l+1)}{2m} \left[\hat{p}_r, \frac{1}{\hat{r}} \right] \\ &\quad + \frac{1}{2m} f^2(\hat{r}) + \frac{2(l+1)\hbar f(\hat{r})}{2m\hat{r}} + \frac{(l+1)^2\hbar^2}{2m\hat{r}^2}, \\ &= \frac{\hat{p}_r^2}{2m} + \frac{\hbar}{2m} f'(\hat{r}) + \frac{f^2(\hat{r})}{2m} + \frac{(l+1)\hbar f(\hat{r})}{m\hat{r}} + \frac{l(l+1)\hbar^2}{2m\hat{r}^2}. \end{aligned} \quad (12.18)$$

$$\therefore V(\hat{r}) - E_{1l} = \frac{\hbar}{2m} f'(\hat{r}) + \frac{f^2(\hat{r})}{2m} + \frac{(l+1)\hbar f(\hat{r})}{m\hat{r}}. \quad (12.19)$$

Equation 12.19 is completely general: to proceed further, $V(\hat{r})$ must be specified.

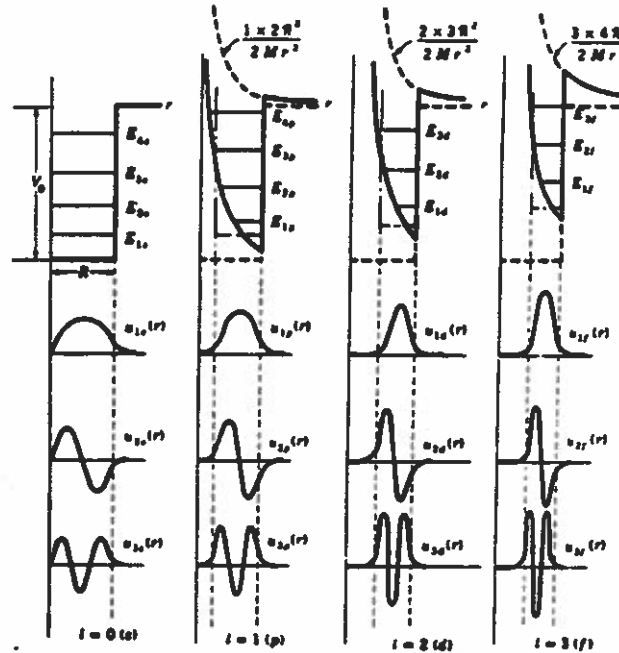


Figure 12.1: Energies and approximate wavefunctions for the finite three-dimensional square well. Solutions are shown for $l = 0, 1, 2, 3$. At the top, the total potential, $W_l(r)$, is shown as a heavy line and the two components, $V(r)$ and $l(l+1)\frac{\hbar^2}{2Mr^2}$, where they differ, are shown as dashed lines. Square wells, similar to these total potentials, are shown as dot-dashed lines: they were used in drawing the wave functions, $u_{nl}(r)$, shown. The energies of the states, shown in the top row, become displaced upwards as the well becomes shallower and narrower. The figure is quantitative and, cf. the text, $M = m$.

12.3 The hydrogen atom central force problem

For an electron in a hydrogen atom:

$$V(\hat{r}) = \frac{-e^2}{4\pi\epsilon_0\hat{r}}, \quad (12.20)$$

where $e = 1.602\,177\,33(49) \times 10^{-19}$ C and $\epsilon_0 = 8.854\,187\,817\dots \times 10^{-12}$ C²·N⁻¹·m⁻²; and

$$f(\hat{r}) = \frac{-me^2}{4\pi\epsilon_0(l+1)\hbar}, \quad (12.21)$$

whence

$$\begin{aligned} V(\hat{r}) - E_{1,l} &= 0 + \frac{1}{2m} \frac{m^2 e^4}{(4\pi\epsilon_0)^2 (l+1)^2 \hbar^2} - \frac{(l+1)\hbar}{m\hat{r}} \frac{me^2}{4\pi\epsilon_0(l+1)\hbar} \\ &= \frac{me^4}{8\epsilon_0^2 \hbar^2 (l+1)^2} - \frac{e^2}{4\pi\epsilon_0\hat{r}} \end{aligned} \quad (12.22)$$

$$\therefore E_{1,l} = \frac{-Ry}{(l+1)^2}, \quad l = 0, 1, 2, \dots, \quad (12.23)$$

where Ry is the Rydberg constant,

$$Ry \equiv \frac{me^4}{8\epsilon_0^2 h^2}. \quad (12.24)$$

For precise energies in hydrogen, Ry must be computed using the reduced mass of the electron, μ_e , for m :

$$\mu_e = \frac{m_e m_p}{m_e + m_p} = \frac{m_e}{1 + \frac{m_e}{m_p}}, \quad (12.25)$$

where m_e and m_p are the rest masses of the electron and proton, respectively,

$$m_e = 9.109\,389\,7(54) \times 10^{-31} \text{ kg}, \quad (12.26)$$

$$m_p = 1.672\,623\,1(10) \times 10^{-27} \text{ kg}, \quad (12.27)$$

$$\frac{m_e}{m_p} = \frac{1}{1836.152\,701(37)}. \quad (12.28)$$

Then, using $h = 6.626\,075\,5(40) \times 10^{-34}$ J·s, the Rydberg constant, $Ry \equiv R_\infty = \frac{\mu_e e^4}{8\epsilon_0^2 h^2}$, is

$$R_\infty = 13.605\,698\,4(40) \text{ eV}, \quad (12.29)$$

and is often given as $R = \frac{R_\infty}{hc}$,

$$R = 10\,973\,731.568\,35(30) \text{ m}^{-1}, \quad (12.30)$$

where R_∞ conveys the effect of using the reduced mass of the system, namely the electron behaves as if it is orbiting a proton of infinite mass.

Equation 12.23 gives the zero-point energy values in each total potential $W_l(\hat{r})$, $l = 0, 1, 2, \dots$. To obtain the energies of the excited states in each $W_l(\hat{r})$ potential, we define

$$A_l^\pm := \frac{1}{\sqrt{2m}} \left\{ \hat{p}_r \mp i \left(f(\hat{r}) + \frac{(l+1)\hbar}{\hat{r}} \right) \right\}; \quad (12.31)$$

then

$$\hat{H}_l - E_{1,l} = A_l^+ A_l^-, \quad (12.32)$$

and we can define

$$\hat{H}_l |1, l\rangle := E_{1,l} |1, l\rangle, \quad (12.33)$$

and

$$A_l^- |1, l\rangle = 0. \quad (12.34)$$

Consider then

$$A_l^+ A_l^- A_l^+ |1, l+1\rangle = (\hat{H}_l - E_{1,l}) A_l^+ |1, l+1\rangle; \quad (12.35)$$

but

$$\begin{aligned}
A_l^- A_l^+ &= \frac{1}{2m} \left\{ \hat{p}_r + i \left(f(\hat{r}) + \frac{(l+1)\hbar}{\hat{r}} \right) \right\} \left\{ \hat{p}_r - i \left(f(\hat{r}) + \frac{(l+1)\hbar}{\hat{r}} \right) \right\} \\
&= \frac{\hat{p}_r^2}{2m} + \frac{i}{2m} \cancel{[f(\hat{r}), \hat{p}_r]} i\hbar f'(\hat{r}) + \frac{i(l+1)\hbar}{2m} \cancel{\left[\frac{1}{\hat{r}}, \hat{p}_r \right]} \frac{-i\hbar}{\hat{r}^2} \\
&\quad + \frac{1}{2m} f^2(\hat{r}) + \frac{2(l+1)\hbar f(\hat{r})}{2m \hat{r}} + \frac{(l+1)^2 \hbar^2}{2m \hat{r}^2} \\
&= \frac{\hat{p}_r^2}{2m} - \frac{\hbar}{2m} f'(\hat{r}) + \frac{1}{2m} f^2(\hat{r}) + \frac{(l+1)\hbar f(\hat{r})}{m \hat{r}} + \frac{(l+1)(l+2)\hbar^2}{2m \hat{r}^2} \quad (12.36) \\
&= A_l^+ A_l^- - \frac{\hbar}{m} f'(\hat{r}) + \frac{(l+1)\hbar^2}{m \hat{r}^2} \\
&= A_l^+ A_l^- - \frac{\hbar}{m} f'(\hat{r}) + \hat{H}_{l+1} - \hat{H}_l \\
&= \hat{H}_{l+1} - \frac{\hbar}{m} f'(\hat{r}) - E_{1,l}.
\end{aligned}$$

$$\therefore A_l^+ A_l^- A_l^+ |1, l+1\rangle = A_l^+ \left(\hat{H}_{l+1} - \frac{\hbar}{m} f'(\hat{r}) - E_{1,l} \right) |1, l+1\rangle, \quad (12.37)$$

$$\therefore (\hat{H}_l - E_{1,l}) A_l^+ |1, l+1\rangle = A_l^+ \left(E_{1,l+1} - \frac{\hbar}{m} f'(\hat{r}) - E_{1,l} \right) |1, l+1\rangle, \quad (12.38)$$

$$\therefore \hat{H}_l A_l^+ |1, l+1\rangle = A_l^+ \left(E_{1,l+1} - \frac{\hbar}{m} f'(\hat{r}) \right) |1, l+1\rangle, \quad (12.39)$$

For an electron in a hydrogen atom, $f'(\hat{r}) = 0$, and

$$\hat{H}_l (A_l^+ |1, l+1\rangle) = E_{1,l+1} (A_l^+ |1, l+1\rangle). \quad (12.40)$$

Thus, we define

$$A_l^+ |1, l+1\rangle := N_{1,l+1}^+ |2, l\rangle, \quad (12.41)$$

where $N_{1,l+1}^+$ is a (normalisation) constant, and

$$E_{1,l+1} := E_{2,l}. \quad (12.42)$$

Reiterating, consider

$$(\hat{H}_l - E_{1,l}) A_l^+ |2, l+1\rangle = A_l^+ A_l^- A_l^+ |2, l+1\rangle, \quad (12.43)$$

$$\therefore (\hat{H}_l - E_{1,l}) A_l^+ |2, l+1\rangle = A_l^+ (\hat{H}_{l+1} - E_{1,l}) |2, l+1\rangle = E_{2,l+1} A_l^+ |2, l+1\rangle. \quad (12.44)$$

Thus, we define

$$A_l^+ |2, l+1\rangle := N_{2,l+1}^+ |3, l\rangle \quad (12.45)$$

and

$$E_{2,l+1} := E_{3,l}. \quad (12.46)$$

Similarly

$$(\hat{H}_l - E_{1,l})A_l^+ |3, l+1\rangle = A_l^+ A_l^- A_l^+ |3, l+1\rangle, \quad (12.47)$$

$$\therefore (\hat{H}_l - E_{1,l})A_l^+ |3, l+1\rangle = A_l^+ (\hat{H}_{l+1} - E_{1,l}) |3, l+1\rangle = E_{3,l+1} A_l^+ |3, l+1\rangle, \quad (12.48)$$

whence

$$A_l^+ |3, l+1\rangle := N_{3,l+1}^+ |4, l\rangle, \quad (12.49)$$

and

$$E_{3,l+1} := E_{4,l}, \quad (12.50)$$

and so on. This process can be depicted as shown in Fig. 12.2. The complete energy eigen-

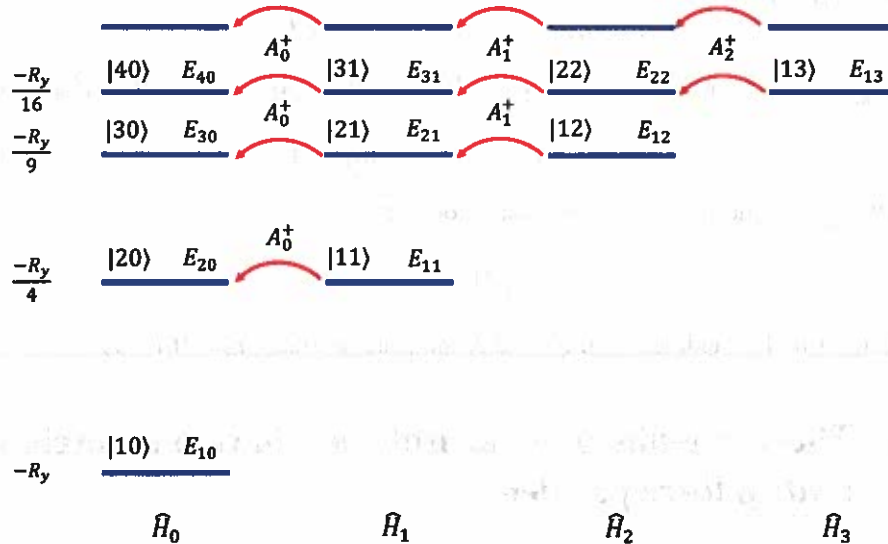


Figure 12.2: The lowest energy eigenstates of the hydrogen atom. The spectrum is grouped by values of the angular momentum quantum number l , reflecting the structure of the total potential, $W_l(\hat{r})$. The energies are given as $-\frac{R_y}{n^2}$, where $R_y = 13.606$ eV and $n = 1, 2, 3, \dots$. The states are labelled by the quantum numbers n_r, l , where $n_r = 1, 2, 3, \dots$ and $n = n_r + l$. The action of the operators A_l^+ is depicted by arrows.

value solution can be stated:

$$E_n = -\frac{R_y}{n^2}, \quad n = 1, 2, 3, \dots, \quad (12.51)$$

where successive energy eigenvalues for a given $\hat{H}_l, l = 0, 1, 2, \dots$, are

$$E_{n_r, l} = \frac{-R_y}{(n_r + l)^2}, \quad n_r = 1, 2, 3, \dots \quad (12.52)$$

i.e.,

$$n := n_r + l. \quad (12.53)$$

A number of features of the result should be noted. First and foremost are the degeneracies in the energy eigenvalues. This result can be viewed from the relationship (cf. eqs. 12.40, 12.44, 12.48)

$$\hat{H}_l(A_l^+ |n_r, l+1\rangle) = E_{n_r, l+1}(A_l^+ |n_r, l+1\rangle), \quad (12.54)$$

and

$$\hat{H}_{l+1}|n_r, l+1\rangle = E_{n_r, l+1}|n_r, l+1\rangle, \quad (12.55)$$

i.e., \hat{H}_l and \hat{H}_{l+1} have the same eigenvalue spectrum (with the exception of the ground state for \hat{H}_l). Such a feature is described: “ \hat{H}_l and \hat{H}_{l+1} are isospectral”. The action of A_l^+ is that of a raising operator:

$$A_l^+ |n_r, l+1\rangle := N_{n_r, l+1}^+ |n_r+1, l\rangle, \quad (12.56)$$

where $N_{n_r, l+1}^+$ is a (normalisation) constant. In turn, the action of A_l^- is that of a lowering operator:

$$A_l^- |n_r+1, l\rangle := N_{n_r+1, l}^- |n_r, l+1\rangle, \quad (12.57)$$

where $N_{n_r+1, l}^-$ is a (normalisation) constant. Note that

$$A_l^- |1, l\rangle = 0. \quad (12.58)$$

This action is understandable from Fig. 12.2: there are no states $|n_r = 0, l+1\rangle$.

12.4 The three-dimensional isotropic harmonic oscillator central force problem

The above development, can also be carried through for a three-dimensional isotropic harmonic oscillator potential, i.e.,

$$V(\hat{r}) = \frac{1}{2}k\hat{r}^2, \quad (12.59)$$

where k is a constant; and

$$f(\hat{r}) = -m\omega\hat{r}, \quad (12.60)$$

where

$$\omega = \sqrt{\frac{k}{m}}. \quad (12.61)$$

Thus, from eq. 12.19

$$\begin{aligned} V(\hat{r}) - E_{1,l} &= -\frac{1}{2}\hbar\omega + \frac{1}{2}m\omega^2\hat{r}^2 - (l+1)\hbar\omega \\ &= -\left(l + \frac{3}{2}\right)\hbar\omega + \frac{1}{2}k\hat{r}^2, \end{aligned} \quad (12.62)$$

$$\therefore E_{1,l} = \left(l + \frac{3}{2}\right)\hbar\omega, \quad l = 0, 1, 2, \dots \quad (12.63)$$

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Further from eq. 12.39

$$\hat{H}_l(A_l^+ |1, l+1\rangle) = A_l^+(E_{1,l+1} + \hbar\omega) |1, l+1\rangle = (E_{1,l+1} + \hbar\omega)(A_l^+ |1, l+1\rangle), \quad (12.64)$$

and so we define

$$A_l^+ |1, l+1\rangle := N_{1,l+1}^+ |2, l\rangle, \quad (12.65)$$

where $N_{1,l+1}^+$ is a (normalisation) constant, and

$$E_{1,l+1} + \hbar\omega := E_{2,l}. \quad (12.66)$$

This process can be reiterated in a manner similar to the hydrogen atom, whence

$$A_l^+ |n_r, l+1\rangle := N_{n_r, l+1}^+ |n_r + 1, l\rangle \quad (12.67)$$

and

$$E_{n_r, l+1} := E_{n_r, l} + \hbar\omega. \quad (12.68)$$

The process can be depicted as shown in Fig. 12.3. The complete energy eigenvalue solution is:

$$E_n = \left(n + \frac{3}{2}\right) \hbar\omega, \quad n = 0, 1, 2, \dots, \quad (12.69)$$

where successive energy eigenvalues for a given \hat{H}_l , $l = 0, 1, 2, \dots$, are

$$E_{n_r, l} = \left\{ 2(n_r - 1) + l + \frac{3}{2} \right\} \hbar\omega, \quad n_r = 1, 2, 3, \dots \quad (12.70)$$

i.e.,

$$n := 2(n_r - 1) + l. \quad (12.71)$$

Compare eq. 12.71 with the corresponding equation (eq. 12.53) for the hydrogen atom. As with the hydrogen atom, there is an isospectral relationship for the three-dimensional isotropic harmonic oscillator, but it is for \hat{H}_{l+2} and \hat{H}_l rather than \hat{H}_{l+1} and \hat{H}_l . Further, as with the hydrogen atom, A_l^+ and A_l^- act as raising and lowering operators: e.g., cf. eqs 12.67 and 12.56; similarly, analogs of eqs. 12.57 and 12.58 exist for the oscillator.

12.5 The three-dimensional isotropic infinite square well central force problem

The above development can also be adapted to obtain the solution for $V(r) = \text{constant}$, where r may be unbounded (free particle) or bounded. For the free particle problem the energy can take any positive value between zero and infinity. Although the operators A_l^+ and A_l^- are not needed to find the energy eigenvalues, they can be used to relate the energy eigenstates for different values of l . It is convenient to work in the position representation. Thus, we seek solutions to

$$H\Psi = E\Psi, \quad (12.72)$$

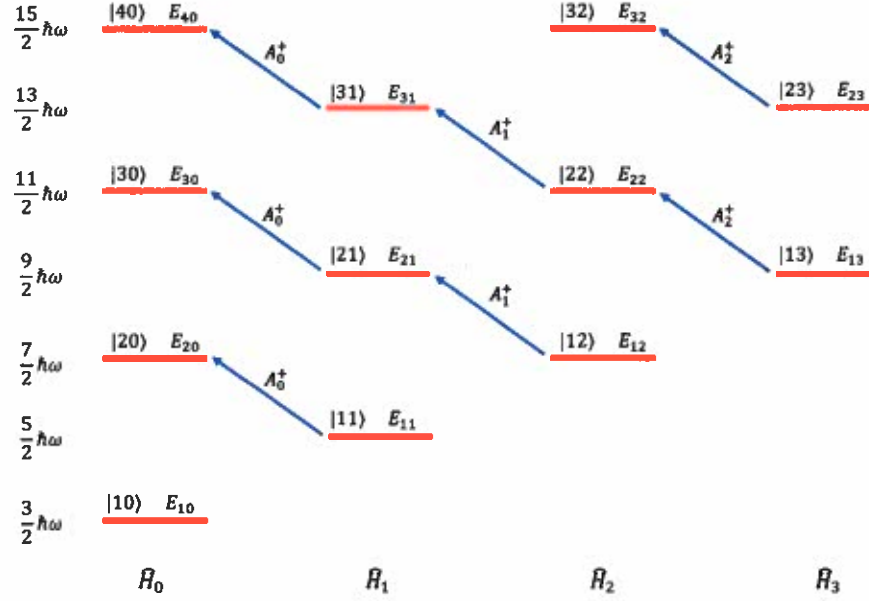


Figure 12.3: The lowest energy eigenstates of the three-dimensional isotropic harmonic oscillator. The spectrum is grouped by values of the angular momentum quantum number l , reflecting the structure of the total potential $W_l(r)$. The energies are given as $(n + \frac{3}{2}\hbar\omega)$, where $\hbar\omega$ is a constant and $n = 0, 1, 2, \dots$. The states are labelled by the quantum numbers n_r, l , where $n_r = 1, 2, 3, \dots$ and $n = 2(n_r - 1) + l$. The action of the operators A_l^{\dagger} is depicted by arrows.

where

$$\Psi := \Psi_{klm}(r, \theta, \phi) = j_l(kr)Y_{lm}(\theta, \phi), \quad k = \sqrt{\frac{2mE}{\hbar}}, \quad (12.73)$$

the $Y_{lm}(\theta, \phi)$ are spherical harmonics, and

$$H := H_l = \frac{p_r^2}{2m} + \frac{l(l+1)\hbar^2}{2mr^2} + (V(r) := 0); \quad (12.74)$$

whence we seek solutions to

$$\left\{ \frac{p_r^2}{2m} + \frac{l(l+1)\hbar^2}{2mr^2} \right\} j_l(kr) = \frac{\hbar^2 k^2}{2m} j_l(kr), \quad (12.75)$$

where

$$p_r = -i\hbar \left(\frac{d}{dr} + \frac{1}{r} \right). \quad (12.76)$$

Consider the special case $l = 0$ for which eq. 12.75 reduces to

$$\frac{-\hbar^2}{2m} \left\{ \frac{d}{dr} + \frac{1}{r} \right\} \left\{ \frac{d}{dr} + \frac{1}{r} \right\} j_0(kr) = \frac{\hbar^2 k^2}{2m} j_0(kr). \quad (12.77)$$

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Equation 12.77 has the solutions:

$$j_0(kr) = \frac{\sin kr}{kr} \quad (12.78)$$

and

$$j_0(kr) = \frac{-\cos kr}{kr}. \quad (12.79)$$

The cosine solution is unphysical because

$$\lim_{r \rightarrow 0} \frac{\cos kr}{kr} = \infty. \quad (12.80)$$

Then, from

$$A_l^- = \frac{1}{\sqrt{2m}} \left\{ p_r + \frac{i\hbar(l+1)}{r} \right\} \quad (12.81)$$

and

$$A_l^+ = \frac{1}{\sqrt{2m}} \left\{ p_r - \frac{i\hbar(l+1)}{r} \right\}, \quad (12.82)$$

it follows that

$$A_l^+ A_l^- = H_l, \quad (12.83)$$

and

$$A_l^- A_l^+ = H_{l+1}. \quad (12.84)$$

Thus,

$$A_l^- A_l^+ A_l^- j_l(kr) = A_l^- H_l j_l(kr) = A_l^- \frac{\hbar^2 k^2}{2m} j_l(kr), \quad (12.85)$$

and so

$$H_{l+1} (A_l^- j_l(kr)) = \frac{\hbar^2 k^2}{2m} (A_l^- j_l(kr)), \quad (12.86)$$

i.e.,

$$A_l^- j_l(kr) \cong j_{l+1}(kr). \quad (12.87)$$

Whence

$$j_{l+1}(kr) \cong \frac{1}{\sqrt{2m}} \left\{ -i\hbar \frac{d}{dr} \frac{-i\hbar}{r} + \frac{i\hbar(l+1)}{r} \right\} j_l(kr), \quad (12.88)$$

$$\therefore j_{l+1}(kr) \cong \left\{ \frac{d}{dr} - \frac{l}{r} \right\} j_l(kr), \quad (12.89)$$

and :

$$\begin{aligned} j_1(kr) &\cong \frac{d}{dr} j_0(kr) = \frac{d}{dr} \left(\frac{\sin kr}{kr} \right) \\ &\cong \frac{k \cos kr}{kr} - \frac{\sin kr}{kr^2} \\ &\cong \frac{\sin kr}{(kr)^2} - \frac{\cos kr}{kr} : \end{aligned} \quad (12.90)$$

$$\begin{aligned}
j_2(kr) &\cong \left\{ \frac{d}{dr} - \frac{1}{r} \right\} \left\{ \frac{\cos kr}{kr} - \frac{\sin kr}{(kr)^2} \right\} \\
&\cong -\frac{k \sin kr}{kr} - \frac{\cos kr}{kr^2} - \frac{k \cos kr}{(kr)^2} + \frac{2k \sin kr}{(kr)^3} - \frac{\cos kr}{kr^2} + \frac{k \sin kr}{(kr)^3} \\
&\cong \frac{3 \sin kr}{(kr)^3} - \frac{3 \cos kr}{(kr)^2} - \frac{\sin kr}{kr};
\end{aligned} \tag{12.91}$$

an so on. The functions $j_l(kr)$ are called the spherical Bessel functions.

For $V(r) = \text{constant}$, the bounded problem is the three-dimensional isotropic square well. The solutions to this problem must be obtained numerically. However, if this well is infinitely deep, i.e.,

$$V(r) = 0, \quad r < R, \tag{12.92}$$

$$V(r) = \infty, \quad r \geq R, \tag{12.93}$$

the solutions are straightforwardly determined: they are fixed by the boundary condition

$$j_l(kR) = 0. \tag{12.94}$$

The solutions to eq. 12.94 are the roots of the spherical Bessel functions. Some of these are given in table 12.1. The corresponding energy eigenvalues are given by

$$E_{nl} = (kR)_{nl}^2 \frac{\hbar^2}{2mR^2}, \tag{12.95}$$

where n, l label the n^{th} root of the spherical Bessel function of order l . These energy eigenvalues are plotted in Fig. 12.4. Note that for $l = 0$ (cf. table 12.1), eq. 12.95 reduces to

$$E_{n0} = \frac{n^2 \hbar^2}{8mR^2}, \tag{12.96}$$

i.e., the energy eigenvalues of the infinite one-dimensional square well. The orbital filling, based on occupancy of the energy eigenstates by spin- $\frac{1}{2}$ particles, is shown. Note the energy gaps for certain particle numbers.

12.6 Exercises

12-1. For the hydrogen atom, the Coulomb plus centrifugal potential is

$$\frac{-e^2}{4\pi\epsilon_0 r} + \frac{l(l+1)\hbar^2}{2mr^2}.$$

For $l = 100$, what is the value of r at the minimum in this potential? [Give your answer in units of $a_0 := 4\pi\epsilon_0\hbar^2/me^2$.]

12-2. An electron moves in a spherically symmetric potential defined by

$$V(r) = -1.00eV, \quad r \leq 10^4 a_0,$$

$$V(r) = 0, \quad r > 10^4 a_0.$$

What is the maximum possible value of l in this potential?

l	$n: 1$	2	3	4	5	6	7
0	π	2π	3π	4π	5π	6π	7π
1	4.4934	7.7253	10.941	14.0662	17.2208	20.3713	
2	5.7635	9.0950	12.3229	15.5146	18.6890	21.8539	
3	6.9879	10.4171	13.6980	16.9236	20.1218		
4	8.1826	11.7049	15.0397	18.3013	21.5254		
5	9.3558	12.9665	16.3547	19.6532			
6	10.5128	14.2074	17.6480	20.9835			
7	11.6570	15.4313	18.9230				
8	12.7908	16.6410	20.1825				
9	13.9158	17.8386	21.4285				
10	15.0335	19.0259					
11	16.1447	20.2039					
12	17.2505	21.3740					
13	18.3513						
14	19.4477						
15	20.5423						
16	21.6292						

Table 12.1: The roots of the spherical Bessel functions: Values $(kR)_{nl}$ for which $j_l(kR) = 0$, where n labels the n^{th} root (values are shown for $(kR)_{nl} < 22$).

12-3. a). Obtain the quantum mechanical version of eq. 12.6, i.e.,

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

b). Using the result from exercise 12-1, obtain eq. 12.9, i.e.,

$$\hat{L}^2 = \hat{r}^2 \hat{p}^2 - (\vec{r}_{op} \cdot \vec{p}_{op})(\vec{r}_{op} \cdot \vec{p}_{op}) + i\hbar(\vec{r}_{op} \cdot \vec{p}_{op}).$$

12.7 Central force problems and so(2,1) or su(1,1) algebra

Recalling eq. 12.14

$$\hat{H} = \frac{\hat{p}_r^2}{2m} + V(\hat{r}) + \frac{l(l+1)}{2m\hat{r}^2} := \hat{H}_l, \quad (12.97)$$

the explicit introduction of the centrifugal potential has effectively reduced the problem to a family of one dimensional problems, each with a different value of l .

General solutions to \hat{H}_l can be explored by considering the commutator bracket algebra of \hat{r} , \hat{p}_r , and polynomials in these operators, where

$$[\hat{r}, \hat{p}_r] = i\hbar. \quad (12.98)$$

We consider only operators of the form

$$\hat{r}^a, \hat{p}_r^b \hat{r}, \hat{r}^c \hat{p}_r^2,$$

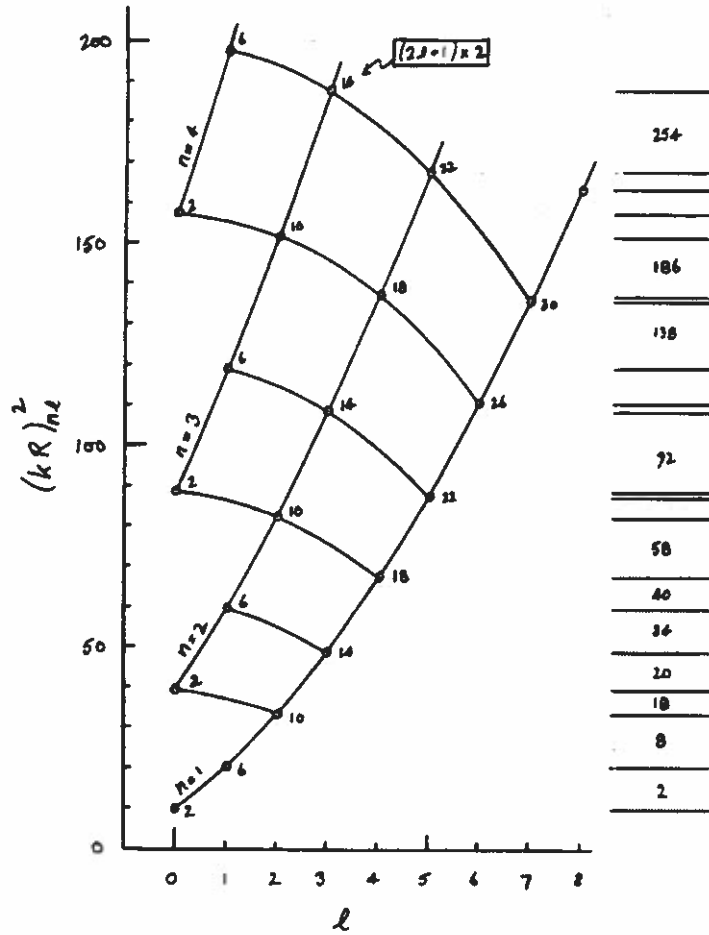


Figure 12.4: The lowest energy eigenstates of the three-dimensional infinite square well. Energies are plotted on the vertical scale, in units of $\frac{\hbar^2}{2mr^2}$ (cf. eq. 12.95). Angular momentum values are plotted on the horizontal scale. The orbital filling, based on m_l and spin- $\frac{1}{2}$ degeneracy ($2 \times (2l + 1)$) is shown.

where a, b and c will be determined by the condition that these operators close under a Lie product (i.e., a commutator-bracket product); and dependence limited to $\hat{p}_r^n, n \leq 2$, is dictated by \hat{H} depending only on \hat{p}_r^2 .

Proceeding (we drop the carets — “^” — from here on, and define $p_r := p$) using

$$[r, p^m] = i\hbar m p^{m-1}, \tag{12.99}$$

$$[r^n, p] = i\hbar n r^{n-1}, \tag{12.100}$$

$$\begin{aligned} [r^a, r^b p] &= r^b [r^a, p] \\ &= i\hbar a r^{a+b-1}. \end{aligned} \tag{12.101}$$

For the algebra to close

$$r^{a+b-1} = r^a, \quad (12.102)$$

whence $b = 1$ and

$$[r^a, rp] = ia\hbar r^a. \quad (12.103)$$

Similarly,

$$[r^a, r^{2-a}p^2] = a(a-1)\hbar^2 + 2ia\hbar rp, \quad (12.104)$$

and

$$[rp, r^{2-a}p^2] = i\hbar ar^{2-a}p^2, \quad (12.105)$$

where the choice $c = 2 - a$ closes the algebra.

Note: these brackets do not depend on a potential and, indeed, we shall explore the freedom in the choice of "a" to describe various potentials.

We introduce a change of variables,

$$V_1 = r^a, \quad (12.106)$$

$$V_2 = \frac{1}{a} \left\{ rp - \frac{1}{2}i(a-1)\hbar \right\}, \quad (12.107)$$

$$V_3 = \frac{1}{a^2} r^{2-a} p^2. \quad (12.108)$$

Then,

$$[V_1, V_2] = i\hbar V_1, \quad (12.109)$$

$$[V_2, V_3] = i\hbar V_3, \quad (12.110)$$

$$[V_3, V_1] = -2i\hbar V_2. \quad (12.111)$$

A subtle and key "extension" of this algebraic structure is realised by noting that "a" can take on both positive and negative values, whence

$$V_1^{-1} = r^{-a} \quad (12.112)$$

yields

$$[V_2, V_1^{-1}] = \frac{1}{a} [rp, r^{-a}] = i\hbar r^{-a} = i\hbar V_1^{-1}. \quad (12.113)$$

$$\therefore [V_2(V_3 + \tau V_1^{-1})] = i\hbar(V_3 + \tau V_1^{-1}), \quad (12.114)$$

where τ is a constant or any operator that commutes with V_1, V_2 and V_3 .

With one further extension of the algebra,

$$T_1 = \frac{1}{2}(V_3 + \tau V_1^{-1} - V_1), \quad (12.115)$$

$$T_2 = V_2, \quad (12.116)$$

$$T_3 = \frac{1}{2}(V_3 + \tau V_1^{-1} + V_1), \quad (12.117)$$

then

$$[T_1, T_2] = -i\hbar T_3, \quad [T_2, T_3] = i\hbar T_1, \quad [T_3, T_1] = i\hbar T_2 \quad (12.118)$$

Consider

$$[T_1, T_2] = i\gamma\hbar T_3, \quad (12.119)$$

$$[T_2, T_3] = i\hbar T_1, \quad (12.120)$$

$$[T_3, T_1] = i\hbar T_2 \quad (12.121)$$

For $\gamma = +1$, this defines the algebra $so(3)$; for $\gamma = -1$, this defines the algebra $so(2, 1)$. [JLW: insert distinction between $so(3)$ and $so(2, 1)$ in terms of preserving geometrical lengths.]

Much of the structure of $so(2, 1)$ can be deduced from our knowledge of $so(3)$:

- 1). Defining raising and lowering operators $T_{\pm} := T_1 \pm iT_2$:

$$[T_+, T_-] = 2\gamma\hbar T_3, \quad (12.122)$$

$$[T_3, T_{\pm}] = \pm\hbar T_{\pm}, \quad (12.123)$$

$$\begin{aligned} T^2 &= \gamma(T_1^2 + T_2^2) + T_3^2 \\ &= \gamma T_+ T_- + T_3^2 - \hbar T_3 \\ &= \gamma T_- T_+ + T_3^2 + \hbar T_3, \end{aligned} \quad (12.124)$$

$$[T^2, T_k] = 0, \quad k = 1, 2, 3. \quad (12.125)$$

- 2). Simultaneous eigenkets of T^2 and T_3 exist and they obey

$$T^2 |Qq\rangle = Q |Qq\rangle, \quad (12.126)$$

$$T_3 |Qq\rangle = q |Qq\rangle, \quad (12.127)$$

$$T_3 T_{\pm} |Qq\rangle = (q \pm \hbar) T_{\pm} |Qq\rangle. \quad (12.128)$$

- 3). The eigenvalues of T_3 are bounded.

Consider

$$\begin{aligned} \langle Qq | (T^2 - T_3^2) |Qq\rangle &= Q - q^2 \\ &= \frac{\gamma}{2} \langle Qq | (T_+ T_- + T_- T_+) |Qq\rangle. \end{aligned} \quad (12.129)$$

This can be rewritten using

$$T_+ |Qq\rangle = |\chi\rangle, \quad T_- |Qq\rangle = |\Psi\rangle, \quad (12.130)$$

whence

$$\frac{1}{2} \langle Qq | (T_+ T_- + T_- T_+) |Qq\rangle = \langle \chi | \chi \rangle + \langle \Psi | \Psi \rangle \geq 0, \quad (12.131)$$

which means, for $\gamma = +1$,

$$Q - q^2 \geq 0, \quad \text{or } q \leq \sqrt{Q}, \quad (12.132)$$

and for $\gamma = -1$,

$$Q - q^2 \leq 0, \quad \text{or } q \geq \pm\sqrt{Q}. \quad (12.133)$$

The eigenvalues of T_3 for $so(3)$ ($T_3 = L_z$) are bounded above and below:

$$q = m_l, \quad m_l = l, l-1, \dots, 1, 0, -1, \dots, -l.$$

The eigenvalues of T_3 for $so(2,1)$ **posses** either an upper bound ($-\sqrt{Q}$) or a lower bound (\sqrt{Q}). (The algebra $so(2,1)$ is termed non-compact.)

- 4). For $so(2,1)$ applied to central force problems we choose the lower bounded case whence a lowest eigenstate is defined

$$T_- |Qq_0\rangle = 0, \quad (12.134)$$

and

$$\begin{aligned} T^2 |Qq_0\rangle &= (-T_+ T_- + T_3^2 - \hbar T_3) |Qq_0\rangle \\ &= q_0(q_0 - \hbar) |Qq_0\rangle. \end{aligned} \quad (12.135)$$

Just as the irreps of $so(3)$ are labeled by l and the eigenvalues of L^2 are $l(l+1)$; so the irreps of $so(2,1)$ are labeled by q_0 and the eigenvalues of T^2 are $q_0(q_0 - \hbar)$. The irreps of $so(2,1)$ are infinite dimensional.

To elucidate the nature of q_0 , consider

$$\begin{aligned} T^2 &= -T_1^2 - T_2^2 + T_3^2 \\ &= (T_3 - T_1)(T_3 + T_1) - [T_3, T_1] - T_2^2 \\ &= V_1(V_3 + \tau V^{-1}) - i\hbar V_2 - V_2^2. \end{aligned} \quad (12.136)$$

Then, using

$$V_2^2 = \frac{1}{a^2} \left\{ r^2 p^2 - ia\hbar r p - \left(\frac{a-1}{2}\right)^2 \hbar^2 \right\}, \quad (12.137)$$

$$\therefore T^2 = \tau + \frac{\hbar^2}{4a^2} (1 - a^2). \quad (12.138)$$

Whence from

$$\langle Qq_0 | T^2 | Qq_0 \rangle = q_0(q_0 - \hbar), \quad (12.139)$$

$$q_0^2 - q_0 \hbar - \left\{ \tau + \frac{\hbar^2}{4a^2} (1 - a^2) \right\} = 0, \quad (12.140)$$

i.e.,

$$q_0 = \frac{\hbar}{2} \left(1 \pm \sqrt{\frac{4\tau}{\hbar^2} + \frac{1}{a^2}} \right). \quad (12.141)$$

12.8 so(2,1) solution for the hydrogen atom

The energy eigenvalue equation for the hydrogen atom is

$$\left\{ \frac{p^2}{2\mu} - \frac{e^2}{4\pi\epsilon_0 r} + \frac{l(l+1)\hbar^2}{2\mu r^2} - E \right\} |Elm_l\rangle = 0. \quad (12.142)$$

Multiply through by $\mu\alpha r$

$$\therefore \left\{ \frac{\alpha r p^2}{2} - \frac{\mu\alpha e^2}{4\pi\epsilon_0} + \frac{\alpha l(l+1)\hbar}{2r} - \mu\alpha r E \right\} |Elm_l\rangle = 0. \quad (12.143)$$

Substituting $\alpha^{-1}r \rightarrow R$, $\alpha p \rightarrow P$

$$\therefore \left\{ \frac{RP^2}{2} - \frac{\mu e^2 \alpha}{4\pi\epsilon_0} + \frac{l(l+1)\hbar}{2R} - \mu\alpha^2 RE \right\} |Elm_l\rangle = 0. \quad (12.144)$$

Then, for

$$V_1 = R, \quad V_2 = RP, \quad V_3 = RP^2 \quad (12.145)$$

this becomes

$$\frac{1}{2} \left\{ V_3 - \frac{\mu e^2 \alpha}{2\pi\epsilon_0} + l(l+1)\hbar^2 V_1^{-1} - 2\mu\alpha^2 V_1 E \right\} |Elm_l\rangle = 0. \quad (12.146)$$

Thus, for

$$(a=1) \quad \tau = l(l+1)\hbar^2, \quad 2\mu\alpha^2 E = -1, \quad q = \frac{\mu e^2 \alpha}{4\pi\epsilon_0} \quad (12.147)$$

$$(T_3 - q) |Elm_l\rangle = 0, \quad (12.148)$$

$$q_0 = \frac{\hbar}{2} \{1 \pm (2l+1)\} = \hbar(l+1), \quad (12.149)$$

$$T^2 = l(l+1)\hbar^2. \quad (12.150)$$

Labelling increments of q by $n_r\hbar$,

$$q = q_0 + n_r\hbar = (l+1)\hbar + n_r\hbar = \frac{\mu e^2 \alpha}{4\pi\epsilon_0}, \quad (12.151)$$

or

$$\alpha = \frac{4\pi\epsilon_0\hbar}{\mu e^2} [(l+1) + n_r], \quad (12.152)$$

$$\therefore E = -\frac{\mu e^4}{32\pi^2\epsilon_0^2\hbar^2 [l+1+n_r]^2} = -\frac{R_y}{n^2}, \quad (12.153)$$

$$\text{where } n = n_r + l + 1. \quad (12.154)$$

Comments

- 1). Each irrep of $so(2,1)$ for the H atom is labeled by a value of l .
- 2). The ladder operators for the H atom change the energy but not l .
- 3). The Hamiltonian for the H atom does not commute with the $so(2,1)$ generators. The algebra $so(2,1)$ is called a spectrum generating algebra of the H atom.

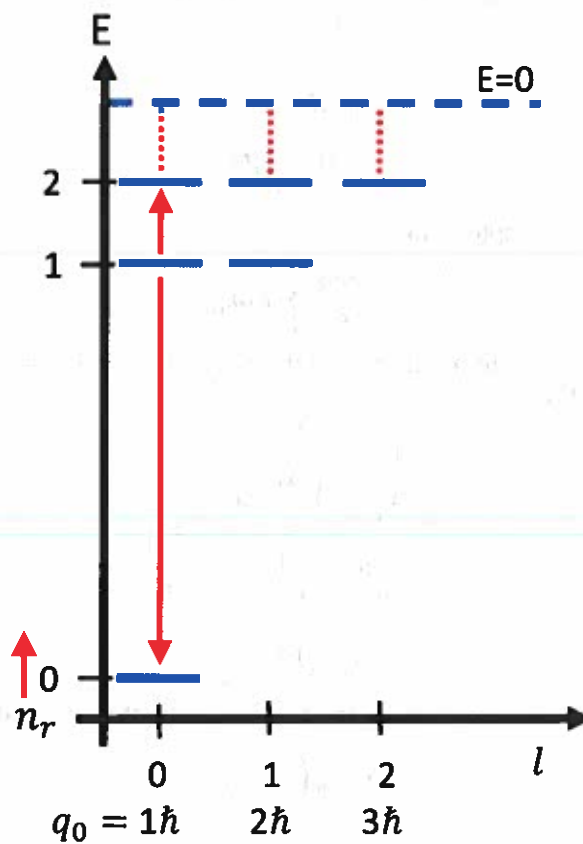


Figure 12.5: The spectrum of the hydrogen atom viewed from the perspective of its $so(2,1)$ algebraic structure.

12.9 so(2,1) solution for the three-dimensional isotropic harmonic oscillator

The energy eigenvalue equation for the three-dimensional isotropic harmonic oscillator is

$$\left\{ \frac{p^2}{2m} + \frac{1}{2}m\omega^2 r^2 + \frac{l(l+1)\hbar^2}{2mr^2} - E \right\} |Elm_l\rangle = 0. \quad (12.155)$$

Multiply through by $\frac{\lambda^2}{4}$ and substitute $R = \lambda^{-1}r$, $P = \lambda p$, yielding

$$\left\{ \frac{P^2}{8m} + \frac{1}{8}m\omega^2 \lambda^4 R^2 + \frac{l(l+1)}{8mR^2} - \frac{\lambda^2 E}{4} \right\} |Elm_l\rangle = 0. \quad (12.156)$$

Then, using eqs. 12.106-12.108, 12.115-12.117, and the condition that $a = 2$,

$$\left\{ \frac{1}{2m} \left(V_3 + \frac{1}{4}m^2\omega^2 \lambda^4 V_1 + \frac{l(l+1)\hbar^2}{4V_1} - \frac{\lambda^2 E}{4} \right) \right\} |Elm_l\rangle = 0. \quad (12.157)$$

Thus, if

$$\frac{1}{4}m^2\omega^2 \lambda^4 := 1, \quad (12.158)$$

$$\tau := \frac{l(l+1)\hbar^2}{4}, \quad (12.159)$$

the eigenvalue equation simplifies to

$$\left\{ T_3 - \frac{\lambda^2 m E}{4} \right\} |Elm_l\rangle = 0. \quad (12.160)$$

The values for the energy are obtained from the eigenvalues of T_3 , once the values for q_0 have been determined, viz.

$$\begin{aligned} q_0 &= \frac{1}{2} \left[\hbar \pm \sqrt{4\tau + \frac{\hbar^2}{a^2}} \right] \\ &= \frac{1}{2} \left[\hbar \pm \hbar \sqrt{l(l+1) + \frac{1}{4}} \right] \\ &= \frac{\hbar^2}{2} \left[1 \pm \left(l + \frac{1}{2} \right) \right]. \end{aligned} \quad (12.161)$$

In anticipation of positive energy values, the positive sign is chosen, yielding

$$q_0 = \frac{\hbar}{2} \left(l + \frac{3}{2} \right). \quad (12.162)$$

Therefore,

$$E = \left(2n_r + l + \frac{3}{2} \right) \hbar \omega, \quad (12.163)$$

or for $N = 2n_r + l$,

$$E = \left(N + \frac{3}{2} \right) \hbar \omega. \quad (12.164)$$

The energy spectrum is given in Fig. 12.6 along with the action of T_+ and T_- .

12.9. $SO(2,1)$ SOLUTION FOR THE THREE-DIMENSIONAL ISOTROPIC HARMONIC OSCILLATOR

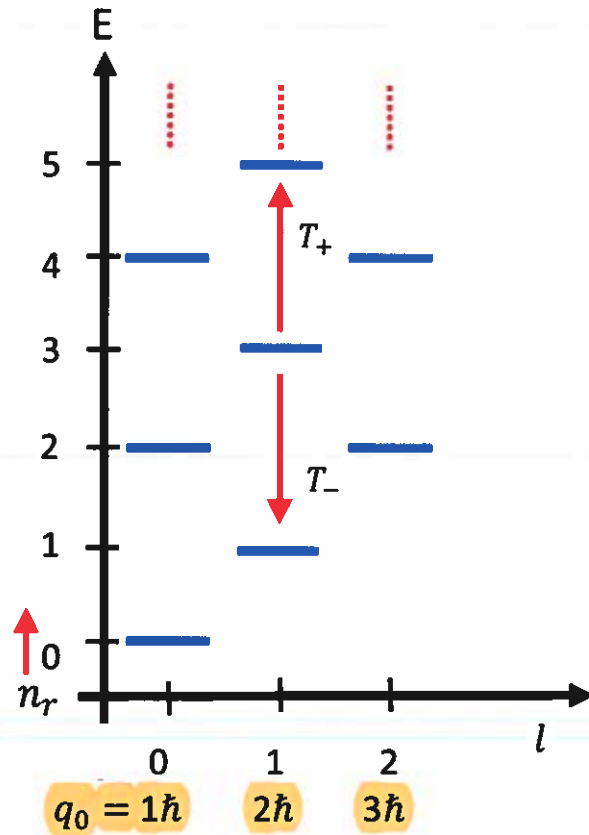


Figure 12.6: The spectrum of the three-dimensional isotropic harmonic oscillator viewed from the perspective of its $so(2,1)$ algebraic structure.

