Complement B_{VII}

A SOLUBLE EXAMPLE OF A CENTRAL POTENTIAL: THE ISOTROPIC THREE-DIMENSIONAL HARMONIC OSCILLATOR

1. Solving the radial equation
2. Energy levels and stationary wave functions

In this complement we shall examine a special case of a central potential for which the radial equation is exactly soluble: the isotropic three-dimensional harmonic oscillator. We have already treated this problem (complement E_V) by considering the state space $\mathcal{E}_r$ as the tensor product $\mathcal{E}_x \otimes \mathcal{E}_y \otimes \mathcal{E}_z$; this amounts, in the $\{ |\mathbf{r}\rangle \}$ representation, to separating the variables in Cartesian coordinates. We thus obtained three differential equations, one in the x-variable, one in y, and the third in z. Here we intend to seek the stationary states which are also eigenstates of $\mathbf{L}^2$ and L_z by separating the variables in polar coordinates. We shall then indicate how the two bases of $\mathcal{E}_r$ obtained by these two different methods are related to each other.

We shall also study, in complement A_{VIII}, the stationary states of well-defined angular momentum of a free particle. This can be considered to be another special case of a central potential $[V(r) \equiv 0]$ which leads to an exactly soluble radial equation.

A three-dimensional harmonic oscillator is composed of a (spinless) particle of mass μ subjected to the potential:

$$V(x, y, z) = \frac{1}{2}\mu[\omega_x^2 x^2 + \omega_y^2 y^2 + \omega_z^2 z^2] \tag{1}$$

where ω_x, ω_y and ω_z are real positive constants. The oscillator is said to be isotropic if:

$$\omega_x = \omega_y = \omega_z = \omega \tag{2}$$

Since the potential (1) is the sum of a function of x alone, a function of y alone and a function of z alone, we can solve the eigenvalue equation of the Hamiltonian:

$$H = \frac{\mathbf{P}^2}{2\mu} + V(\mathbf{R}) \tag{3}$$

by separating the variables x, y and z in the $\{ |\mathbf{r}\rangle \}$ representation. This is what was done in complement E_V. The energy levels, for an isotropic oscillator, are then found to be of the form:

$$E_n = \left(n + \frac{3}{2}\right)\hbar\omega \tag{4}$$

where n is any positive integer or zero. The degree of degeneracy g_n of the level E_n is equal to:

$$g_n = \frac{1}{2}(n+1)(n+2) \tag{5}$$

and the associated eigenfunctions are:

$$\varphi_{n_x,n_y,n_z}(x, y, z) = \left(\frac{\beta^2}{\pi}\right)^{3/4} \frac{1}{\sqrt{2^{n_x+n_y+n_z}\, n_x!\, n_y!\, n_z!}} e^{-\frac{\beta^2}{2}(x^2+y^2+z^2)} \times H_{n_x}(\beta x)\, H_{n_y}(\beta y)\, H_{n_z}(\beta z) \tag{6}$$

with:

$$\beta = \sqrt{\frac{\mu\omega}{\hbar}} \tag{7}$$

[$H_p(u)$ denotes the Hermite polynomial of degree p; *cf.* complement B_V]. φ_{n_x,n_y,n_z} is an eigenfunction of the Hamiltonian H with the eigenvalue E_n such that:

$$n = n_x + n_y + n_z \tag{8}$$

If the oscillator under consideration is isotropic*, the potential (1) is a function only of the distance r between the particle and the origin:

$$V(r) = \frac{1}{2}\mu\omega^2 r^2 \tag{9}$$

Consequently, the three components of the orbital angular momentum $\mathbf{L}$ are constants of the motion. We want to find the common eigenstates of H, $\mathbf{L}^2$ and L_z. To do so, we could proceed, as in complement D_{VI}, by introducing operators related to right and left circular quanta and to "longitudinal" quanta corresponding to the third degree of freedom along Oz (an outline of this method is given at the end of this complement). However, we prefer to use this example to illustrate the method elaborated in chapter VII (§ A) and solve the radial equation by the polynomial method.

1. Solving the radial equation

For a fixed value of the quantum number l, the radial functions $R_{k,l}(r)$ and energies $E_{k,l}$ are given by the equation:

$$\left[-\frac{\hbar^2}{2\mu}\frac{1}{r}\frac{d^2}{dr^2}r + \frac{1}{2}\mu\omega^2 r^2 + \frac{l(l+1)\hbar^2}{2\mu r^2}\right] R_{k,l}(r) = E_{k,l}\, R_{k,l}(r) \tag{10}$$

* Separation of the polar variables r, θ, φ is possible only for an isotropic oscillator.

We set:

$$R_{k,l}(r) = \frac{1}{r} u_{k,l}(r) \tag{11-a}$$

$$\varepsilon_{k,l} = \frac{2\mu E_{k,l}}{\hbar^2} \tag{11-b}$$

Equation (10) then becomes:

$$\left[\frac{d^2}{dr^2} - \beta^4 r^2 - \frac{l(l+1)}{r^2} + \varepsilon_{k,l}\right] u_{k,l}(r) = 0 \tag{12}$$

[where β is the constant defined in (7)]. We must add the condition at the origin:

$$u_{k,l}(0) = 0 \tag{13}$$

For large r, (12) virtually reduces to:

$$\left[\frac{d^2}{dr^2} - \beta^4 r^2\right] u_{k,l}(r) \underset{r\to\infty}{\simeq} 0 \tag{14}$$

The asymptotic behavior of the solutions of equation (12) is therefore dominated by $e^{\beta^2 r^2/2}$ or $e^{-\beta^2 r^2/2}$. Only the second possibility is physically acceptable. This leads us to the change of functions:

$$u_{k,l}(r) = e^{-\beta^2 r^2/2} y_{k,l}(r) \tag{15}$$

It is easy to find that $y_{k,l}(r)$ must satisfy:

$$\frac{d^2}{dr^2} y_{k,l} - 2\beta^2 r \frac{d}{dr} y_{k,l} + \left[\varepsilon_{k,l} - \beta^2 - \frac{l(l+1)}{r^2}\right] y_{k,l} = 0 \tag{16-a}$$

$$y_{k,l}(0) = 0 \tag{16-b}$$

Now we shall seek $y_{k,l}(r)$ in the form of a power series in r:

$$y_{k,l}(r) = r^s \sum_{q=0}^{\infty} a_q r^q \tag{17}$$

where, by definition, a_0 is the coefficient of the first non-zero term:

$$a_0 \neq 0 \tag{18}$$

When we substitute expansion (17) into equation (16-a), the term of lowest order is in r^{s-2}; its coefficient is zero if:

$$[s(s-1) - l(l+1)]a_0 = 0 \tag{19}$$

With conditions (18) and (16-b) taken into account, the only way to satisfy relation (19) is to choose:

$$s = l + 1 \tag{20}$$

(this result could have been predicted; *cf.* § A-2-c of chapter VII). The next term in the expansion of equation (16-a) is in r^{s-1}, and its coefficient is equal to:

$$[s(s+1) - l(l+1)]a_1 \tag{21}$$

Since s is already fixed by (20), this coefficient can go to zero only if:

$$a_1 = 0 \tag{22}$$

Finally, let us set the coefficient of the general term in r^{q+s} equal to zero:

$$[(q+s+2)(q+s+1) - l(l+1)]\,a_{q+2} + [\varepsilon_{k,l} - \beta^2 - 2\beta^2(q+s)]\,a_q = 0 \tag{23}$$

that is, using (20):

$$(q+2)(q+2l+3)\,a_{q+2} = [(2q+2l+3)\beta^2 - \varepsilon_{k,l}]\,a_q \tag{24}$$

We therefore obtain a recurrence relation for the coefficients a_q of expansion (17).

Note, first of all, that this recurrence relation, combined with result (22), implies that *all coefficients a_q of odd rank q are zero*. As for the coefficients of even rank, they must all be proportional to a_0. If the value of $\varepsilon_{k,l}$ is such that no integer q makes the term in brackets on the right-hand side of (24) go to zero, we find the solution $y_{k,l}$ of (16) in the form of an infinite power series, for which:

$$\frac{a_{q+2}}{a_q} \underset{q\to\infty}{\sim} \frac{2\beta^2}{q} \tag{25}$$

This behavior is the same as that of the coefficients appearing in the expansion of the function $e^{\beta^2 r^2}$, since:

$$e^{\beta^2 r^2} = \sum_{p=0}^{\infty} c_{2p}\, r^{2p} \tag{26}$$

with:

$$c_{2p} = \frac{\beta^{2p}}{p!} \tag{27}$$

and, consequently:

$$\frac{c_{2p+2}}{c_{2p}} \underset{p\to\infty}{\sim} \frac{\beta^2}{p} \tag{28}$$

Since it is $2p$ which corresponds to the even integer q of the expansion of $y_{k,l}$, (28) is indeed identical to (25). From this, we can see that if (17) really contains an infinite number of terms, the asymptotic behavior of $y_{k,l}$ is dominated by $e^{\beta^2 r^2}$, which renders this function physically unacceptable [*cf.* relation (15)].

The only cases which are interesting from a physical point of view are therefore those in which there exists an even integer k, positive or zero, such that:

$$\varepsilon_{k,l} = (2k + 2l + 3)\beta^2 \tag{29}$$

Recurrence relation (24) indicates that the coefficients of even rank greater than k are then zero. Since all the coefficients of odd rank are also zero, expansion (17) reduces to a polynomial, and the radial function $u_{k,l}(r)$ given by (15) decreases exponentially as r goes to infinity.

2. Energy levels and stationary wave functions

Using definitions (7) and (11-b), relation (29) gives the energies $E_{k,l}$ associated with a given value of l:

$$E_{k,l} = \hbar\omega\left(k + l + \frac{3}{2}\right) \tag{30}$$

where k is any even positive integer or zero. Since $E_{k,l}$ actually depends only on the sum:

$$n = k + l \tag{31}$$

accidental degeneracies appear: the energy levels of the isotropic three-dimensional harmonic oscillator are of the form:

$$E_n = \left(n + \frac{3}{2}\right)\hbar\omega \tag{32}$$

l is any positive integer or zero, and k is any even positive integer or zero; n can therefore take on all integral values, positive or zero. This is in agreement with result (4).

We shall fix an energy E_n, that is, an integer n, positive or zero. The values of k and l which can be associated with it according to (31) are the following:

$$(k, l) = (0, n), \quad (2, n-2), \ldots (n-2, 2), \quad (n, 0) \qquad \text{if } n \text{ is even} \tag{33-a}$$

$$(k, l) = (0, n), \quad (2, n-2), \ldots (n-3, 3), \quad (n-1, 1) \qquad \text{if } n \text{ is odd} \tag{33-b}$$

From this, we can immediately get the values of l associated with the first values of n:

$$\begin{aligned} &n = 0: \quad l = 0 \\ &n = 1: \quad l = 1 \\ &n = 2: \quad l = 0, 2 \\ &n = 3: \quad l = 1, 3 \\ &n = 4: \quad l = 0, 2, 4 \end{aligned} \tag{34}$$

Figure 1 represents, with the same conventions as for the hydrogen atom (*cf.* figure 4 of chapter VII), the lowest energy levels of an isotropic three-dimensional harmonic oscillator.

For each pair (k, l), there exists one and only one radial function $u_{k,l}(r)$, that is, $(2l + 1)$ common eigenfunctions of H, $\mathbf{L}^2$ and L_z:

$$\varphi_{k,l,m}(\mathbf{r}) = \frac{1}{r} u_{k,l}(r)\, Y_l^m(\theta, \varphi) \tag{35}$$

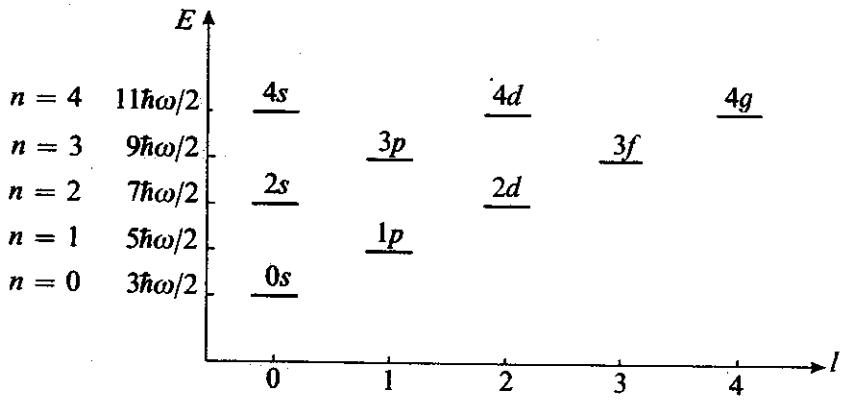

FIGURE 1

Lowest energy levels of the three-dimensional harmonic oscillator. When n is even, l can take on $\frac{n}{2}+1$ values: $l = n, n-2, \ldots 0$. When n is odd, l can take on $\frac{n+1}{2}$ values: $l = n, n-2, \ldots 1$. With the possible values of $m(-l \leqslant m \leqslant l)$ taken into account, the degree of degeneracy of the level E_n is $\frac{(n+1)(n+2)}{2}$.

Consequently, the degree of degeneracy of the energy E_n under consideration is equal to:

$$g_n = \sum_{l=0,2,\cdots,n} (2l+1) \qquad \text{if } n \text{ is even} \tag{36-a}$$

$$g_n = \sum_{l=1,3,\cdots,n} (2l+1) \qquad \text{if } n \text{ is odd} \tag{36-b}$$

These sums are simple to calculate, and we again obtain result (5):

$$\text{for even } n: \quad g_n = \sum_{p=0}^{n/2} (4p+1) = \frac{1}{2}(n+1)(n+2) \tag{37-a}$$

$$\text{for odd n}: \quad g_n = \sum_{p=0}^{(n-1)/2} (4p+3) = \frac{1}{2}(n+1)(n+2) \tag{37-b}$$

For each of the pairs (k, l) given in (33), the results of §1 enable us to determine the corresponding radial function $u_{k,l}(r)$ (to within the factor a_0) and, therefore, the $(2l+1)$ common eigenfunctions of H and $\mathbf{L}^2$, of eigenvalues E_n and $l(l+1)\hbar^2$. We shall calculate, for example, the wave functions associated in this way with the three lowest energy levels.

For the ground state $E_0 = \frac{3}{2}\hbar\omega$, we must have:

$$k = l = 0 \tag{38}$$

$y_{0,0}(r)$ then reduces to $a_0 r$. If we choose a_0 to be real and positive, the normalized function $\varphi_{k=l=m=0}$ can be written:

$$\varphi_{0,0,0}(\mathbf{r}) = \left(\frac{\beta^2}{\pi}\right)^{3/4} e^{-\beta^2 r^2/2} \tag{39}$$

Since the ground state is not degenerate ($g_0 = 1$), $\varphi_{0,0,0}$ is the same as the function $\varphi_{n_x=n_y=n_z=0}$ which is found by separating the Cartesian variables x, y, and z [*cf.* formula (6)].

With the first excited state $\left(E_1 = \frac{5}{2}\hbar\omega\right)$, which is three-fold degenerate, is again associated a single pair (k, l):

$$\begin{cases} k = 0 \\ l = 1 \end{cases} \tag{40}$$

and $y_{0,1} = a_0 r^2$. The three functions of the basis defined by $\mathbf{L}^2$ and L_z are therefore :

$$\varphi_{0,1,m}(\mathbf{r}) = \sqrt{\frac{8}{3}} \frac{\beta^{3/2}}{\pi^{1/4}} \beta r \, e^{-\beta^2 r^2/2} Y_1^m(\theta, \varphi) \qquad m = 1, 0, -1 \tag{41}$$

We know [*cf.* complement A_{VI}, formulas (32)] that the spherical harmonics Y_1^m are such that:

$$\begin{aligned} rY_1^0(\theta, \varphi) &= \sqrt{\frac{3}{4\pi}} z \\ \frac{r}{\sqrt{2}}[Y_1^{-1} - Y_1^1] &= \sqrt{\frac{3}{4\pi}} x \\ \frac{r}{\sqrt{2}}[Y_1^{-1} + Y_1^1] &= -i\sqrt{\frac{3}{4\pi}} y \end{aligned} \tag{42}$$

and that the Hermite polynomial of order 1 is [*cf.* complement B_V, formulas (18)] :

$$H_1(u) = 2u \tag{43}$$

Consequently, it is clear that the three functions $\varphi_{0,1,m}$ are related to the functions φ_{n_x,n_y,n_z} of basis (6) by the equations:

$$\begin{aligned} \varphi_{n_x=0,n_y=0,n_z=1} &= \varphi_{k=0,l=1,m=0} \\ \varphi_{n_x=1,n_y=0,n_z=0} &= \frac{1}{\sqrt{2}}[\varphi_{k=0,l=1,m=-1} - \varphi_{k=0,l=1,m=1}] \\ \varphi_{n_x=0,n_y=1,n_z=0} &= \frac{i}{\sqrt{2}}[\varphi_{k=0,l=1,m=-1} + \varphi_{k=0,l=1,m=1}] \end{aligned} \tag{44}$$

Finally, consider the second excited state, of energy $E_2 = \frac{7}{2}\hbar\omega$. It is six-fold degenerate, and the quantum numbers k and l can take on the values:

$$k = 0, \quad l = 2 \tag{45-a}$$

$$k = 2, \quad l = 0 \tag{45-b}$$

The function $y_{0,2}(r)$ which corresponds to the values (45-a) is simply $a_0 r^3$. For the values (45-b), $y_{2,0}$ contains two terms; using (24) and (29), we easily find :

$$y_{2,0}(r) = a_0 r\left[1 - \frac{2}{3}\beta^2 r^2\right] \tag{46}$$

The six basis functions in the eigensubspace associated with E_2 are thus of the form:

$$\varphi_{0,2,m}(\mathbf{r}) = \sqrt{\frac{16}{15}} \frac{\beta^{3/2}}{\pi^{1/4}} \beta^2 r^2 \, e^{-\beta^2 r^2/2} \, Y_2^m(\theta, \varphi) \qquad m = 2, 1, 0, -1, -2 \quad (47\text{-a})$$

$$\varphi_{2,0,0}(\mathbf{r}) = \sqrt{\frac{3}{2}} \frac{\beta^{3/2}}{\pi^{3/4}} \left(1 - \frac{2}{3} \beta^2 r^2\right) e^{-\beta^2 r^2/2} \quad (47\text{-b})$$

Knowing the explicit expressions for the spherical harmonics [formulas (33) of complement A_{VI}] and the Hermite polynomials [formulas (18) of complement B_V], we can easily prove the following relations:

$$\varphi_{k=2,l=0,m=0} = -\frac{1}{\sqrt{3}} [\varphi_{n_x=2,n_y=0,n_z=0} + \varphi_{n_x=0,n_y=2,n_z=0} + \varphi_{n_x=0,n_y=0,n_z=2}]$$

$$\frac{1}{\sqrt{2}} [\varphi_{k=0,l=2,m=2} + \varphi_{k=0,l=2,m=-2}]$$

$$= \frac{1}{\sqrt{2}} [\varphi_{n_x=2,n_y=0,n_z=0} - \varphi_{n_x=0,n_y=2,n_z=0}]$$

$$\frac{1}{\sqrt{2}} [\varphi_{k=0,l=2,m=2} - \varphi_{k=0,l=2,m=-2}] = i \varphi_{n_x=1,n_y=1,n_z=0}$$

$$\frac{1}{\sqrt{2}} [\varphi_{k=0,l=2,m=1} - \varphi_{k=0,l=2,m=-1}] = -\varphi_{n_x=1,n_y=0,n_z=1}$$

$$\frac{1}{\sqrt{2}} [\varphi_{k=0,l=2,m=1} + \varphi_{k=0,l=2,m=-1}] = -i \varphi_{n_x=0,n_y=1,n_z=1}$$

$$\varphi_{k=0,l=2,m=0} = \sqrt{\frac{2}{3}} [\varphi_{n_x=0,n_y=0,n_z=2} - \frac{1}{2} \varphi_{n_x=2,n_y=0,n_z=0}$$

$$- \frac{1}{2} \varphi_{n_x=0,n_y=2,n_z=0}] \quad (48)$$

COMMENT:

As we pointed out in the beginning of this complement, we can apply a method analogous to the one presented in complement D_{VI} to the isotropic three-dimensional harmonic oscillator. If a_x, a_y and a_z are the annihilation operators which act in the state spaces $\mathcal{E}_x$, $\mathcal{E}_y$ and $\mathcal{E}_z$ respectively, we define:

$$a_d = \frac{1}{\sqrt{2}} (a_x - i a_y) \quad (49\text{-a})$$

$$a_g = \frac{1}{\sqrt{2}} (a_x + i a_y) \quad (49\text{-b})$$

If can be shown that a_d and a_g behave like independent annihilation oper-

ators (complement D_{VI}, §3-b). The Hamiltonian H and the angular momentum operators can then be expressed in terms of a_d, a_g, a_z and their adjoints:

$$H = \hbar\omega\left(N_d + N_g + N_z + \frac{3}{2}\right) \tag{50-a}$$

$$L_z = \hbar(N_d - N_g) \tag{50-b}$$

$$L_+ = \hbar\sqrt{2}\,(a_z^\dagger a_g - a_d^\dagger a_z) \tag{50-c}$$

$$L_- = \hbar\sqrt{2}\,(a_g^\dagger a_z - a_z^\dagger a_d) \tag{50-d}$$

The common eigenvectors $|\chi_{n_d,n_g,n_z}\rangle$ of the observables N_d, N_g and N_z can be obtained through the action of the creation operators $a_d^\dagger$, $a_g^\dagger$ and $a_z^\dagger$ on the ground state $|0, 0, 0\rangle$ of the Hamiltonian H [this state is unique to within a constant factor; *cf.* formulas (6) and (39)]:

$$|\chi_{n_d,n_g,n_z}\rangle = \frac{1}{\sqrt{n_d!\,n_g!\,n_z!}}(a_d^\dagger)^{n_d}(a_g^\dagger)^{n_g}(a_z^\dagger)^{n_z}\,|0, 0, 0\rangle \tag{51}$$

According to (50-a) and (50-b), $|\chi_{n_d,n_g,n_z}\rangle$ is an eigenvector of H and L_z with the eigenvalues $(n_d + n_g + n_z + 3/2)\hbar\omega$ and $(n_d - n_g)\hbar$. The eigensubspace $\mathscr{E}_n$ associated with a given energy E_n can therefore be spanned by the set of vectors $|\chi_{n_d,n_g,n_z}\rangle$ such that:

$$n_d + n_g + n_z = n \tag{52}$$

Of these, the eigenvector of L_z with the largest eigenvalue compatible with E_n is $|\chi_{n,0,0}\rangle$, whose eigenvalue is $n\hbar$. This ket, according to (50-c), satisfies:

$$L_+\,|\chi_{n,0,0}\rangle = 0 \tag{53}$$

Consequently*, it is an eigenvector of $\mathbf{L}^2$ with the eigenvalue $n(n+1)\hbar^2$, and it can be identified with the ket of the $\{|\varphi_{k,l,m}\rangle\}$ basis such that:

$$\begin{aligned} &k + l = n \\ &l = m = n \end{aligned} \tag{54}$$

Therefore:

$$|\varphi_{k=0,l=n,m=n}\rangle = |\chi_{n_d=n,n_g=0,n_z=0}\rangle \tag{55}$$

Application of the operator L_- [formula (50-d)] to both sides of relation (55) yields:

$$|\varphi_{0,n,n-1}\rangle = -\,|\chi_{n-1,0,1}\rangle \tag{56}$$

* This result follows directly from relation (C-7-b) of chapter VI, which, applied to $|\chi_{n,0,0}\rangle$, yields:

$$\mathbf{L}^2\,|\chi_{n,0,0}\rangle = \hbar^2(n^2 + n)\,|\chi_{n,0,0}\rangle$$

The eigenvalue $(n-2)\hbar$ of L_z, unlike the two preceding ones, is two-fold degenerate in $\mathscr{E}_n$: two orthogonal vectors, $|\chi_{n-2,0,2}\rangle$ and $|\chi_{n-1,1,0}\rangle$ correspond to it. Using (50-d) again in order to apply L_- to (56), we find that:

$$|\varphi_{0,n,n-2}\rangle = \sqrt{\frac{2(n-1)}{2n-1}}\,|\chi_{n-2,0,2}\rangle - \frac{1}{\sqrt{2n-1}}\,|\chi_{n-1,1,0}\rangle \tag{57}$$

It can be shown that the action of L_+ on the linear combination orthogonal to (57) yields the null vector. This linear combination must therefore be an eigenvector of $\mathbf{L}^2$ with the eigenvalue $(n-2)(n-1)\hbar^2$. This gives, to within a phase factor:

$$|\varphi_{2,n-2,n-2}\rangle = \frac{1}{\sqrt{2n-1}}\,|\chi_{n-2,0,2}\rangle + \sqrt{\frac{2(n-1)}{2n-1}}\,|\chi_{n-1,1,0}\rangle \tag{58}$$

We can thus relate, by iteration*, the two bases, $\{|\chi_{n_d,n_g,n_z}\rangle\}$ and $\{|\varphi_{k,l,m}\rangle\}$. Of course, replacing $a_d^\dagger$ and $a_g^\dagger$ by functions of $a_x^\dagger$ and $a_y^\dagger$ in (51), we can express $|\chi_{n_d,n_g,n_z}\rangle$ as a linear combination of the vectors $|\varphi_{n_x,n_y,n_z}\rangle$ whose wave functions are given by (6).

References and suggestions for further reading:

Other soluble examples (spherical square well, etc.): Messiah (1.17), chap. IX, §10; Schiff (1.18), §15; see also Flügge (1.24), §§58 to 79.

* An argument analogous to the one just outlined will be used in chapter X to add two angular momenta.