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The Harmonic Oscillator in Modern Physics

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and

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The fourth part (chapters VIII, IX, and X) deals respectively with four-, five-, and six-dimensional oscillators and their application to the Coulomb problem, the Bohr–Mottelson collective nuclear model, and the Interacting Boson Model (IBM). All that is required for their understanding is presented in previous sections — in particular chapter VII, with the exception of section 42 where some more advanced group theoretical notions are needed.

Finally, the fifth part (chapters XI, XII, and XIII) deals with the relativistic many body problems with oscillator interactions, though the discussion is mainly restricted to systems of one, two, and three particles and applied to the mass spectra of mesons (quark–antiquark systems) and baryons (three quark systems). Knowledge of the elements of the special theory of relativity and, in quantum mechanics, of the Dirac and Klein–Gordon equations, is assumed, though otherwise this part is again self-contained.

In the Conclusions we stress that we have touched only on some aspects of the harmonic oscillator in modern physics related to our own work, or to that of those with whom we have come in personal contact.

Chapter I

The One-Body Problem

1 The Radial Wave Function of the Harmonic Oscillator

We begin by recalling some results that may be found in any elementary quantum-mechanics text. The time-independent Schrödinger equation for the harmonic oscillator in units in which, $\hbar, m$ and the frequency of the oscillator are equal to 1 becomes

$$(-\tfrac{1}{2}\nabla^2 + \tfrac{1}{2}r^2)\psi = E\psi. \tag{1.1}$$

Assuming a solution of the form

$$\psi = \frac{\phi(r)}{r} e^{-\frac{1}{2}r^2} Y_{lm}(\vartheta, \varphi) \equiv \psi_{nlm}(\mathbf{x}) = \langle \mathbf{x}|nlm\rangle \equiv |nlm\rangle, \tag{1.2}$$

where $Y_{lm}(\theta, \varphi)$ are the spherical harmonics, we have for ϕ the equation

$$-\phi'' + 2r\phi' + \phi + \frac{l(l+1)}{r^2}\phi = 2E\phi. \tag{1.3}$$

We give in (1.2) the different notations we shall use in these lectures for the single-particle harmonic oscillator states. The index n appearing in them is justified below.

If we try a power-series solution for ϕ,

$$\phi = r^p \sum_{k=0}^{\infty} a_k r^k, \tag{1.4}$$

we obtain a recursion relation between the a_k:

$$\frac{a_{k+2}}{a_k} = -\frac{(2E-1)-2(p+k)}{(p+k+2)(p+k+1)-l(l+1)}. \tag{1.5}$$

Let $k = -2, a_{-2} = 0$; then $p(p-1) = l(l+1)$ and hence $p = l+1$, as $p = -l$ is unacceptable because ϕ would diverge at $r = 0$.

We must truncate the series (1.4) at some $k_{\max}$ as this series even when multiplied by $\exp(-\frac{1}{2}r^2)$ does not converge when $r \to \infty$. Thus,

$$2E - 1 - 2(p + k_{\max}) = 0. \tag{1.6}$$

Since $k_{\max}$ must be even, let $k_{\max} = 2n$. Then,

$$E = 2n + l + \tfrac{3}{2}, \tag{1.7}$$

and the normalized solution to the radial equation is

$$R_{nl}(r) \equiv \frac{\phi(r)}{r} e^{-\frac{1}{2}r^2} = r^l \sum_{k=0}^{n} a_{nlk} r^{2k} e^{-\frac{1}{2}r^2}, \tag{1.8}$$

where it may be shown from (1.5) that [1]

$$a_{nlk} = \frac{(-1)^k}{k!} \left[\frac{2(n!)}{\Gamma(n+l+\frac{3}{2})}\right]^{\frac{1}{2}} \frac{\Gamma(n+l+\frac{3}{2})}{(n-k)!\Gamma(k+l+\frac{3}{2})}. \tag{1.9}$$

2 The Matrix Elements of $f(r)Y_{\lambda\mu}(\theta,\varphi)$ with Respect to Harmonic Oscillator States. The Coefficients $B(n'l', nl, p)$

Suppose we wish to find the matrix elements, with respect to states of the harmonic oscillator, of $f(r)Y_{\lambda\mu}(\theta,\varphi)$ where $Y_{\lambda\mu}(\theta,\varphi)$ is a spherical harmonic, *i.e.*, an irreducible Racah tensor of order λ and component μ. From (1.2) and (1.8), the matrix element separates into an angular part and a radial part:

$$\begin{aligned}
&\langle n'l'm'|f(r)Y_{\lambda\mu}(\theta,\varphi)|nlm\rangle \\
&\quad = \int\int\int R_{n'l'}(r)Y^*_{l'm'}(\theta,\varphi)f(r)Y_{\lambda\mu}(\theta,\varphi) \\
&\qquad \times R_{nl}(r)Y_{lm}(\theta,\varphi)r^2 \sin\theta\, dr d\theta d\varphi \qquad (2.1)\\
&\quad = \int_0^\infty R_{n'l'}(r)f(r)R_{nl}(r)r^2 dr \langle l'm'|Y_{\lambda\mu}(\theta,\varphi)|lm\rangle.
\end{aligned}$$

By the Wigner-Eckart theorem and the analysis given in Rose [2] one obtains

$$\langle l'm'|Y_{\lambda\mu}(\theta,\varphi)|lm\rangle = (-1)^{m'}\sqrt{\tfrac{(2l+1)(2l'+1)(2\lambda+1)}{4\pi}} \begin{pmatrix} l & \lambda & l' \\ m & \mu & -m' \end{pmatrix} \begin{pmatrix} l & \lambda & l' \\ 0 & 0 & 0 \end{pmatrix}, \tag{2.2}$$

where $\begin{pmatrix} l & \lambda & l' \\ m & \mu & -m' \end{pmatrix}$ is a $3j$ coefficient. We may evaluate the radial integral by substituting the explicit form (1.8) of R_{nl} into (2.1) and get

$$\int_0^\infty R_{n'l'}(r)f(r)R_{nl}(r)r^2 dr = \sum_{k=0}^{n}\sum_{k'=0}^{n'} a_{nlk}a_{n'l'k'} \int_0^\infty r^{2k+2k'+l+l'} f(r)e^{-r^2}r^2 dr. \tag{2.3}$$

Define

$$p \equiv \tfrac{1}{2}(2k + 2k' + l + l'). \tag{2.4}$$

Note that p ranges from $\frac{1}{2}(l+l')$ to $\frac{1}{2}(l+l') + n + n'$, and the last term in (2.2) implies, from parity considerations, that p is integer (half-integer) if λ is even (odd). Solving for k' we get $k' = p - k - \frac{1}{2}(l+l')$. We may now rewrite (2.3) as

$$\sum_p\sum_k a_{nlk}a_{n'l'p-k-\frac{1}{2}(l+l')} \int_0^\infty r^{2p+2} f(r)e^{-r^2} dr \equiv \sum_p B(n'l', nl, p)I_p, \tag{2.5}$$

where we have defined the B coefficients by

$$B(n'l', nl, p) \equiv \tfrac{1}{2}\Gamma(p+\tfrac{3}{2}) \sum_k a_{nlk}a_{n'l'p-k-\frac{1}{2}(l+l')}, \tag{2.6}$$

and I_p is a Talmi integral [3] defined by

$$I_p \equiv \frac{2}{\Gamma(p+\frac{3}{2})} \int_0^\infty r^{2p+2} f(r)e^{-r^2} dr. \tag{2.7}$$

The normalization in (2.7) is chosen so that for $f(r) = 1, I_p = 1$. The coefficients $B(n'l', nl, p)$ have been discussed and tabulated by Brody and Moshinsky [1,4].

The matrix element (2.1) reduces to

$$
\begin{aligned}
&\langle n'l'm'|f(r)Y_{\lambda\mu}(\theta,\varphi)|nl\acute{m}\rangle \\
&\quad = \sum_p B(n'l', nl, p) I_p (-1)^{m'} \sqrt{\frac{(2l+1)(2l'+1)(2\lambda+1)}{4\pi}} \\
&\quad \times \begin{pmatrix} l & \lambda & l' \\ m & \mu & -m' \end{pmatrix} \begin{pmatrix} l & \lambda & l' \\ 0 & 0 & 0 \end{pmatrix} .
\end{aligned}
\tag{2.8}
$$

For convenience we tabulate here the most common Talmi integrals:

$f(r)$	I_p	
r^λ	$\frac{\Gamma(p+\frac{1}{2}\lambda+\frac{3}{2})}{\Gamma(p+\frac{3}{2})}$	(2.9)
$\dfrac{e^{-\mu r}}{\mu r}$	$\frac{2e^{\mu^2/4}}{\mu\Gamma(p+\frac{3}{2})} \int_{\mu/2}^{\infty} (x-\frac{1}{2}\mu)^{2p+1} e^{-x^2} dx$	(2.10)
$e^{-\alpha^2 r^2}$	$(1+\alpha^2)^{-p-3/2}$	(2.11)
$\dfrac{1}{r}$	$\frac{p!}{\Gamma(p+\frac{3}{2})}$	(2.12)

The first one appears when we are dealing with problems involving electric multipoles in which case we have to compute the matrix elements of $r^\lambda Y_{\lambda\mu}(\theta,\varphi)$. The next two appear in nuclear problems when we assume Yukawa or Gaussian interaction between two nucleons. The last one appears for a Coulomb interaction.

3 The One-Electron Atomic Problem. Variational Analysis of the Ground State of the Hydrogen Atom in Terms of Harmonic Oscillator States

All calculations in nuclear physics have two important flaws: (1) one does not use a complete set of basis functions but rather, by introducing models, restricts the basis sufficiently to make calculations feasible; (2) the nuclear Hamiltonian is not known with the precision of other fields in physics.

If the results of calculations differ from experiment, it is not apparent which of the two flaws is at fault. This problem does not exist in atomic or molecular problems, where the Hamiltonian is known exactly. There, if calculations do not agree with experiment, we have made a bad choice in the selection of the basis functions. We shall therefore apply frequently in these lectures harmonic oscillator states to the description of n–electron atoms or molecules, both for its intrinsic interest and for the insight to the approximation procedure.

We shall neglect the spin-orbit interaction. It is a relativistic effect and, for atoms and molecules of few electrons, is small. The Hamiltonian for a system of n electrons and N nuclei is

$$
\begin{aligned}
H' = {} & \textstyle\sum_{s=1}^{n} \frac{(p'_s)^2}{2m} + \sum_{s<t=2}^{n} \frac{e^2}{|\mathbf{x}'_s - \mathbf{x}'_t|} - \sum_{\alpha=1}^{N} \sum_{s=1}^{n} \frac{Z_\alpha e^2}{|\mathbf{x}'_s - \mathbf{X}'_\alpha|} \\
& + \textstyle\sum_{\alpha<\beta=2}^{N} \frac{Z_\alpha Z_\beta e^2}{|\mathbf{X}'_\alpha - \mathbf{X}'_\beta|} ,
\end{aligned}
\tag{3.1}
$$

where $\mathbf{x}'_s$ is the position vector of the sth electron, $\mathbf{X}'_\alpha$ is the position vector of the αth nucleus and Z_α is the charge of nucleus α. The last term in (3.1) gives the repulsion between nuclei and — in the Born-Oppenheimer approximation in which the nuclei are fixed — it is a constant. The constant vectors $\mathbf{X}'_\alpha$ will enter the calculation as variational parameters.

As a trial wave function we shall use a harmonic oscillator wave function of a certain frequency ω, which will be a variational parameter.

Make the change of variables

$$
\left.
\begin{aligned}
x_{is} &= \sqrt{\left(m\omega/\hbar\right)} x'_{is} \\
X_{i\alpha} &= \sqrt{\left(m\omega/\hbar\right)} X'_{i\alpha} \\
p_{is} &= (m\omega\hbar)^{-1/2} p'_{is} \\
H &= \left(me^4/2\hbar^2\right)^{-1} H'
\end{aligned}
\right\} ,
\tag{3.2}
$$

where $\frac{1}{2}me^4/\hbar^2 \equiv E_B$ is the energy of the first Bohr orbit.

Define a dimensionless parameter

$$
\epsilon \equiv \sqrt{\frac{\hbar\omega}{E_B}} = \sqrt{\left[\hbar\omega \Big/ \left(\frac{me^4}{2\hbar^2}\right)\right]} .
\tag{3.3}
$$

Then,

$$
H = \tfrac{1}{2}\epsilon^2 \textstyle\sum_{s=1}^{n} (p_s)^2 + \sqrt{2}\epsilon \Bigg[\sum_{s<t=2}^{n} \frac{1}{|\mathbf{X}_s - \mathbf{X}_t|}
$$

$$-\textstyle\sum_{\alpha=1}^{N}\sum_{s=1}^{n}\frac{Z_\alpha}{|\mathbf{x}_s-\mathbf{X}_\alpha|}+\sum_{\alpha<\beta=2}^{N}\frac{Z_\alpha Z_\beta}{|\mathbf{X}_\alpha-\mathbf{X}_\beta|}\Big]. \tag{3.4}$$

In the case of the hydrogen atom $N = n = 1$ and we choose $X_\alpha = 0$, *i.e.*, we put the nucleus at the origin. Then,

$$H = \tfrac{1}{2}\epsilon^2 p^2 - \sqrt{2}\epsilon\frac{1}{r}, \tag{3.5}$$

where $r = |\mathbf{x}|$.

The eigenstates ψ of (3.5) have definite l, m and so we could expand them in terms of the corresponding states ψ_{nlm} of (1.2) of the harmonic oscillator, *i.e.*,

$$\psi = \sum_n a_n|nlm\rangle. \tag{3.6}$$

For a variational analysis of the energy we calculate $\int \psi^* H\psi d\tau$ and minimize this, subject to the constraint $\int \psi^*\psi d\tau = 1$, *i.e.*,

$$\delta\left[\int \psi^* H\psi d\tau - \lambda\int \psi^*\psi d\tau\right] = 0. \tag{3.7}$$

As from (3.6) ψ is linear in the a's, this is equivalent to diagonalising $\|\int \psi^*_{n'lm} H\psi_{nlm} d\tau\|$ for fixed l, m. The lowest eigenvalue, when minimized with respect to ϵ, will be the energy predicted by the variational procedure for the above trial wave function. As

$$H_{\text{ho}} = \tfrac{1}{2}(p^2 + r^2), \tag{3.8}$$

which implies

$$\tfrac{1}{2}p^2 = H_{\text{ho}} - \tfrac{1}{2}r^2, \tag{3.9}$$

then

$$\begin{aligned}\langle n'lm|H|nlm\rangle &= \langle n'lm\Big|\Big(\epsilon^2 H_{\text{ho}} - \tfrac{1}{2}\epsilon^2 r^2 - \sqrt{2}\epsilon\frac{1}{r}\Big)\Big|nlm\rangle\\ &= \epsilon^2(2n+l+\frac{3}{2})\delta_{n'n} - \tfrac{1}{2}\epsilon^2\int_0^\infty R_{n'l}(r)r^4R_{nl}(r)dr\\ &\quad -\sqrt{2}\epsilon\int_0^\infty R_{n'l}(r)\frac{1}{r}R_{nl}(r)r^2dr.\end{aligned} \tag{3.10}$$

For the first integral we use the recurrence relations of associate Laguerre polynomials [5]. The second integral may be expanded in terms of Talmi integrals and, using (2.12), we obtain

$$\begin{aligned}&\langle n'lm|H|nlm\rangle\\ &= \tfrac{1}{2}\epsilon^2\Big\{[n(n+l+\tfrac{1}{2})]^{\frac{1}{2}}\delta_{n'n-1} + (2n+l+\tfrac{3}{2})\delta_{n'n}\\ &\qquad +[(n+1)(n+l+\tfrac{3}{2})]^{\frac{1}{2}}\delta_{n'n+1}\Big\}\\ &\qquad -\sqrt{2}\epsilon\sum_{p=l}^{l+n+n'} B(n'l,nl,p)\frac{p!}{\Gamma(p+\frac{3}{2})}.\end{aligned} \tag{3.11}$$

The ground state of the H atom has $l = m = 0$. We need then to calculate the matrix $\|\langle n'00|H|n00\rangle\|$. For up to $\mathfrak{N}$ quanta, we would have to diagonalize a $(\frac{1}{2}\mathfrak{N}+1)\times(\frac{1}{2}\mathfrak{N}+1)$ matrix, *i.e.*, $n = 0, 1, \ldots, \frac{1}{2}\mathfrak{N}$. Suppose we limit ourselves to zero quanta ($n = n' = 0$); then from the Tables [4] of coefficients B we find

$$\langle H\rangle \equiv \langle 000|H|000\rangle = \frac{3}{4}\epsilon^2 - \sqrt{2}\epsilon B(00,00,0)\frac{1}{\Gamma(\frac{3}{2})} = \frac{3}{4}\epsilon^2 - \sqrt{2}\epsilon\frac{2}{\sqrt{\pi}}. \tag{3.12}$$

Minimizing $\langle H\rangle$ with respect to ϵ we get

$$\frac{\partial}{\partial\epsilon}\left[\frac{3}{4}\epsilon^2 - 2\sqrt{\frac{2}{\pi}}\epsilon\right] = \frac{3}{2}\epsilon - 2\sqrt{\frac{2}{\pi}} = 0, \tag{3.13}$$

$$\epsilon = \frac{4}{3}\sqrt{\frac{2}{\pi}} = 1.06. \tag{3.14}$$

From (3.3) $\epsilon = \sqrt{(\hbar\omega/E_B)}$ where $E_B = 13.6$ eV. Thus,

$$\hbar\omega = (1.06)^2 E_B. \tag{3.15}$$

Using the value (3.14) for ϵ the energy is

$$\langle 000|H|000\rangle = -\frac{4}{3}\times\frac{2}{\pi} = -0.849 \tag{3.16}$$

in units of the energy of the first Bohr orbit. Note that this is greater than $-E_B$ as it must be.

If we do the same thing for $\mathfrak{N}$ quanta, keeping ϵ fixed at 1.06, we get [6]

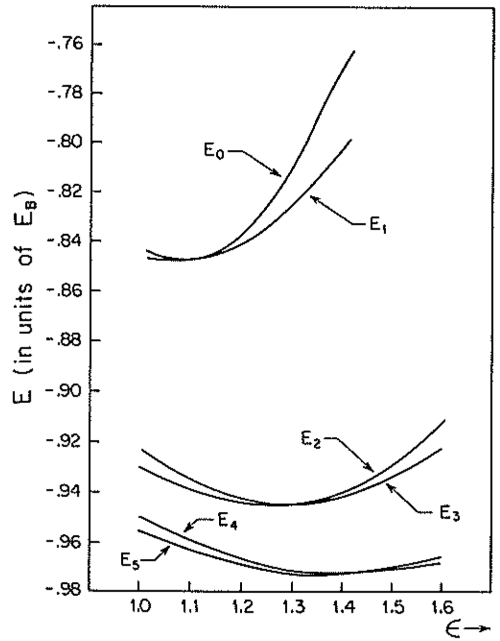

Figure I.1. Energy of the ground state of the H atom as a function of the parameter ϵ for the variational analysis discussed in Section 3. This energy $E_p(\epsilon)$, $p = 0, 1, 2, 3, 4, 5$ is associated with a trial wave function $\psi_p = \sum_{n=0}^{p} a_n^{(p)} |n00\rangle$, where $|n00\rangle$ is a harmonic-oscillator state of frequency $\hbar\omega = (me^4/2\hbar^2)\epsilon^2$.

Number of quanta	Percentage of binding energy
0	84.9%
2	84.9%
4	93.33%
6	93.73%
8	95.75%
10	96.19%

If — for ten quanta — we vary ϵ, the accuracy increases to 97.35%.

The dependence of the binding energy on ϵ may be seen [7] from Fig. I.1 in which the energies $E_{\mathfrak{N}/2}$ for the $\mathfrak{N}$–quantum approximation are plotted as a function of ϵ in units of the energy of the first Bohr orbit. As one increases the number of quanta, the value of ϵ for which the binding energy is minimum increases. In other words, the frequency of the harmonic oscillator for which we get the minimum is increasing.

Note also that the dramatic improvement in the binding energy occurs when one increases the number of quanta by four, rather than by two. This is a general property observed in many calculations [7,8] which we shall prove here rigorously for an arbitrary potential $V(r')$ when we consider its variational analysis for states with $l = m = 0$ and 0+2 quanta, *i.e.*, $n = 0, 1$. The Hamiltonian can then be written as

$$H = \frac{1}{2m}p'^2 + V(r') = \tfrac{1}{2}\hbar\omega p^2 + V\left(\left[\frac{\hbar}{m\omega}\right]^{\frac{1}{2}} r\right), \tag{3.17}$$

and its matrix with respect to the above states is

$$\begin{pmatrix} \langle 000|H|000\rangle & \langle 000|H|100\rangle \\ \langle 100|H|000\rangle & \langle 100|H|100\rangle \end{pmatrix}, \tag{3.18}$$

where

$$\begin{aligned}\langle 000|H|000\rangle &= \frac{3}{4}\hbar\omega + \frac{4}{\sqrt{\pi}}\int_0^\infty r^2 V\left(r\sqrt{\frac{\hbar}{m\omega}}\right)e^{-r^2}dr \\ &= \frac{3}{4}\hbar\omega + \frac{4}{\sqrt{\pi}}\int_0^\infty \left(\frac{m\omega}{\hbar}\right)^{\frac{3}{2}} r'^2 V(r')\exp\left(-\frac{m\omega}{\hbar}r'^2\right)dr',\end{aligned} \tag{3.19}$$

$$\begin{aligned}\langle 100|H|000\rangle &= \tfrac{1}{2}\sqrt{\frac{3}{2}}\hbar\omega + \sqrt{\frac{3}{2}}\frac{4}{\sqrt{\pi}}\int_0^\infty r^2 V\left(r\sqrt{\frac{\hbar}{m\omega}}\right)e^{-r^2}dr \\ &\quad - \sqrt{\frac{3}{2}}\frac{8}{3\sqrt{\pi}}\int_0^\infty r^4 V\left(r\sqrt{\frac{\hbar}{m\omega}}\right)e^{-r^2}dr,\end{aligned} \tag{3.20}$$

and a similar expression for $\langle 100|H|100\rangle$, all of which can be obtained using the tables of coefficients B of reference [4]. We shall now take the derivative of $\langle 000|H|000\rangle$, with respect to $\hbar\omega$ and see immediately from (3.19) and (3.20) that

$$\frac{d}{d(\hbar\omega)}\langle 000|H|000\rangle = \sqrt{\frac{3}{2}}\frac{1}{\hbar\omega}\langle 100|H|000\rangle. \tag{3.21}$$

It is clear therefore that for the frequency $\hbar\omega$ for which $\langle 000|H|000\rangle$ is a minimum, *i.e.*, when (3.21) is zero, we have also $\langle 100|H|000\rangle = 0$; so that there is no improvement for the binding energy when we go from 0 to 0+2 quanta at this frequency. More general relations of this type have been derived by Dubovoy and Flores [8].

4 The One-Electron Molecular Problem. The Ground State of H_2^+ in Terms of Harmonic Oscillator States

From (3.4) we see that the one-electron molecular problem has the Hamiltonian

$$H = \tfrac{1}{2}\epsilon^2 p^2 - \sqrt{2}\epsilon\left[\sum_{\alpha=1}^{N}\frac{Z_\alpha}{|\mathbf{x}-\mathbf{X}_\alpha|} - \sum_{\alpha<\beta=2}^{N}\frac{Z_\alpha Z_\beta}{|\mathbf{X}_\alpha - \mathbf{X}_\beta|}\right]. \tag{4.1}$$

For the discussion of the matrix elements of H with respect to harmonic oscillator states $|nlm\rangle$ we need only analyse the matrix element of $|\mathbf{x}-\mathbf{X}|^{-1}$ with respect to these states when $\mathbf{X}$ is some fixed vector. Denoting by (r,θ,φ) and (R,Θ,Φ) the coordinates of $\mathbf{x}$ and $\mathbf{X}$ respectively, and using the expansion

$$\frac{1}{|\mathbf{x}-\mathbf{X}|} = \sum_{k=0}^{\infty}\begin{bmatrix} r^k/R^{k+1} \\ R^k/r^{k+1}\end{bmatrix}\frac{4\pi}{2k+1}\sum_{q=-k}^{k} Y^*_{kq}(\Theta,\Phi)Y_{kq}(\theta,\varphi), \tag{4.2}$$

where upper (lower) terms in the square brackets are employed according to whether $r \leq R (r > R)$, the matrix element of $|\mathbf{x}-\mathbf{X}|^{-1}$ reduces to a linear combination of matrix elements of the form

$$\begin{aligned}
&\langle n'l'm'\left|\begin{bmatrix} r^k/R^{k+1} \\ R^k/r^{k+1}\end{bmatrix} Y_{kq}(\theta,\varphi)\right|nlm\rangle \\
&= \langle n'l'\left\|\begin{bmatrix} r^k/R^{k+1} \\ R^k/r^{k+1}\end{bmatrix} Y_k(\theta,\varphi)\right\|nl\rangle(-1)^{l-k+m'} \\
&\quad\times\sqrt{2l'+1}\begin{pmatrix} l & k & l' \\ m & q & -m'\end{pmatrix} \\
&= \sum_p\left\{B(n'l',nl,p)I_p^k(R)(-1)^{m'}\begin{pmatrix} l & k & l' \\ m & q & -m'\end{pmatrix}\right. \\
&\quad\left.\times\begin{pmatrix} l & k & l' \\ 0 & 0 & 0\end{pmatrix}\sqrt{\frac{(2l+1)(2l'+1)(2k+1)}{4\pi}}\right\},
\end{aligned} \tag{4.3}$$

where

$$\begin{aligned}
I_p^k(R) &\equiv \frac{2}{\Gamma(p+\frac{3}{2})}\left[\int_0^R \frac{r^{2p+k+2}}{R^{k+1}}e^{-r^2}dr + \int_R^\infty R^k r^{2p-k+1}e^{-r^2}dr\right] \\
&= \frac{1}{\Gamma(p+\frac{3}{2})}\left\{\left[\sum_{q=0}^{p-\frac{1}{2}k} R^{2q+k}\frac{(p-\frac{1}{2}k)!}{q!}\right.\right.
\end{aligned}$$

$$\begin{aligned}
&\left.-\sum_{q=0}^{p+\frac{1}{2}k}\frac{R^{2q-k}}{2^{p-q+\frac{1}{2}k}}\frac{(2p+k+1)!!}{(2q+1)!!}\right]e^{-R^2} \\
&\left.+\frac{\sqrt{\pi}(2p+k+1)!!}{R^{k+1}2^{p+1+\frac{1}{2}k}}\operatorname{erf}(R)\right\}.
\end{aligned} \tag{4.4}$$

In (4.4) $\operatorname{erf}(R)$ stands for the error function

$$\operatorname{erf}(R) \equiv \frac{2}{\sqrt{\pi}}\int_0^R e^{-t^2}dt. \tag{4.5}$$

From the selection rule implied by the coefficient $\begin{pmatrix} l & k & l' \\ 0 & 0 & 0\end{pmatrix}$ in Eq. (4.3), *i.e.*, $l + l' + k$ even, and from the restriction on the values of p implied in (2.4), we conclude that $p \pm \frac{1}{2}k$ in (4.4) is always an integer.

Particularizing the Hamiltonian (4.1) to the H_2^+ molecule, we could take the two protons with coordinates $\mathbf{X}_1 = \mathbf{X}, \mathbf{X}_2 = -\mathbf{X}$, $\mathbf{X}$ being a vector along the z-axis of magnitude, R, $2R$ being the intermolecular distance. If we then take the expectation value of H with respect to a zero-quantum harmonic oscillator state, we obtain

$$\langle H\rangle = \langle 000|H|000\rangle = \frac{3}{4}\epsilon^2 + \epsilon f(R), \tag{4.6}$$

with

$$f(R) = \frac{1}{R\sqrt{2}}[1 - 4\operatorname{erf}(R)]. \tag{4.7}$$

We shall choose for ϵ the value that minimizes $\langle H\rangle$ when we take for R the value R_0 which gives the lowest value for $\langle H\rangle$, *i.e.*, ϵ and R_0 are determined by the equations

$$\frac{\partial}{\partial\epsilon}\langle H\rangle = \frac{3}{2}\epsilon + f(R) = 0, \quad \frac{\partial}{\partial R}\langle H\rangle = \epsilon\frac{df}{dR} = 0. \tag{4.8}$$

The value R_0 is obtained by drawing $f(R)$ and seeking its minimum, while ϵ is given by $\epsilon = -\frac{2}{3}f(R_0)$. Thus we finally get for $\langle H\rangle$ the expression

$$\langle H\rangle_{\min} \equiv E(R) = \frac{1}{3}f(R_0)[f(R_0) - 2f(R)]. \tag{4.9}$$

In Fig. I.2 we give $E(R)$ for H_2^+ as compared with the exact calculation. The total electronic energy we get at the minimum of the curve is 84% of

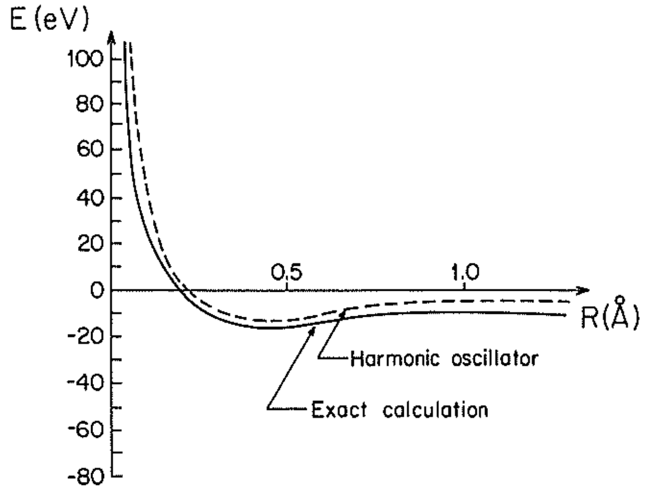

Figure I.2. Expectation value $E(R)$ of the Hamiltonian of the H_2^+ molecule as a function of R, half the internuclear distance. The single-electron wave function is represented by a zero-quantum state of the harmonic oscillator, whose frequency is chosen so as to minimize the energy $E(R)$.

the experimental value and the theoretical internuclear distance is 1.022 Å, while the experimental one is 1.06 Å.

For H_2^+ Bender [9] has carried out calculations with harmonic oscillator functions of up to four quanta. In his analysis he deals with electronic energies, *i.e.*, he does not include the term of nuclear repulsion. Taking the results of Bender for the experimental $R = 0.53$ Å with the value for the frequency of the oscillator that minimizes the energy for the given R, and adding $e^2/2R$, one gets the following:

(a) The calculated energy for the state $|000\rangle$ is 84% of the experimental one, coinciding with the above analysis, as of course it should.

(b) For a linear combination of the states $|000\rangle$ and $|100\rangle$ the calculated energy is 88.66% of the exact value.

(c) For a linear combination of $|000\rangle$ and $|020\rangle$ the calculated energy is 88.88% of the exact value.

(d) For the following combination

$$a_1|000\rangle + a_2|100\rangle + a_3|020\rangle + a_4|200\rangle + a_5|120\rangle + a_6|040\rangle, \tag{4.10}$$

which corresponds to an approximation of up to four quanta, one gets from Bender's analysis 93.46% of the exact energy and the following values for the coefficients:

$$\left.\begin{array}{lll} a_1 = 0.96396 & a_3 = 0.15880 & a_5 = 0.06226 \\ a_2 = -0.18707 & a_4 = 0.07847 & a_6 = 0.02334 \end{array}\right\} . \tag{4.11}$$

We see that the convergence with increasing number of quanta for H_2^+ is as good as for H.

5 Scattering of Electrons by Hydrogen Atoms and the Form Factor of the Electron-Charge Distribution in the Ground State

We have used harmonic oscillator states for a variational analysis of the ground state of the hydrogen atom. In the following sections we shall employ them in the analysis of the form factor of the hydrogen atom to establish the basis for a similar analysis later on of the form factor of the ^3H nucleus considered as a three nucleon system and of the α particle as a four-nucleon system.

We first indicate how one could derive experimentally the form factor from the differential elastic scattering cross section of electrons by hydrogen atoms. For high (but still non-relativistic) energies the differential scattering cross section could be given by the Born approximation [10]*

$$d\sigma = \frac{m^2}{4\pi^2\hbar^4}\left|\int U(r')\exp(i\mathrm{q}\cdot\mathrm{r}')d\mathrm{r}'\right|^2 d\Omega, \tag{5.1}$$

where m is the electron mass, $d\Omega$ the differential solid angle and $\hbar\mathrm{q}$ the momentum transfer

$$\hbar\mathrm{q} = \mathrm{p}' - \bar{\mathrm{p}}',$$

or, as $p' = \bar{p}'$,

$$\hbar q = 2p'\sin\tfrac{1}{2}\theta, \tag{5.2}$$

---

*We use always r', p', etc. to indicate coordinates and momenta in ordinary units and reserve r, p for the corresponding dimensionless quantities.

where θ is the scattering angle. In (5.1) $U(r')$ can be taken as the sum of the potential due to the proton plus the one due to the electron charge distribution, *i.e.*,

$$U(r') = -\frac{e^2}{r'} + e^2 \int \frac{\rho(\mathbf{r}'')}{|\mathbf{r}' - \mathbf{r}''|} d\mathbf{r}'', \tag{5.3}$$

where $\rho(\mathbf{r}')$ is given in terms of the ground state wave function ψ by

$$\rho(\mathbf{r}') = \psi^*(\mathbf{r}')\psi(\mathbf{r}'). \tag{5.4}$$

Making use of the convolution theorem [11] that states

$$\int dx e^{ikx} \int dy f(x-y) g(y) = \int dx e^{ikx} f(x) \int dy e^{iky} g(y), \tag{5.5}$$

we obtain

$$\begin{aligned} \frac{d\sigma}{d\Omega} &= \frac{m^2}{4\pi^2\hbar^4} \left| \int \left[\frac{e^2}{r'} - \int \frac{e^2 \rho(\mathbf{r}'')}{|\mathbf{r}' - \mathbf{r}''|} d\mathbf{r}'' \right] \exp(i\mathbf{q}\cdot\mathbf{r}') d\mathbf{r}' \right|^2 \\ &= \left(\frac{d\sigma}{d\Omega}\right)_R \left| 1 - \int \rho(\mathbf{r}') \exp(i\mathbf{q}\cdot\mathbf{r}') d\mathbf{r}' \right|^2, \end{aligned} \tag{5.6}$$

where

$$\left(\frac{d\sigma}{d\Omega}\right)_R = \frac{m^2}{4\pi^2\hbar^4} \left| \int \frac{e^2}{r'} \exp(i\mathbf{q}\cdot\mathbf{r}') d\mathbf{r}' \right|^2 \tag{5.7}$$

is the Rutherford scattering cross section.

From (5.6) we see that

$$1 - \left[\left(\frac{d\sigma}{d\Omega}\right) \Big/ \left(\frac{d\sigma}{d\Omega}\right)_R \right]^{\frac{1}{2}} = \int \rho(\mathbf{r}') \exp(i\mathbf{q}\cdot\mathbf{r}') d\mathbf{r}' \equiv F(\mathbf{q}), \tag{5.8}$$

where $F(\mathbf{q})$ is the form factor for the electron charge distribution in the ground state of the hydrogen atom. From the experimental information on the ratio of the differential elastic cross section to the Rutherford differential cross section, we can therefore obtain information on $F(\mathbf{q})$ and, from (5.8) and (5.4), on the ground-state wave function $\psi(\mathbf{r}')$.

Of course, in the case of the hydrogen atom we know the wave function for the ground state:

$$\psi(r') = \frac{1}{\sqrt{(\pi a^3)}} \exp\left(-\frac{r'}{a}\right), \tag{5.9}$$

where $a = \hbar^2/me^2$ is the Bohr radius; so the exact form factor $F_e(\mathbf{q})$ is

$$\begin{aligned} F_e(\mathbf{q}) &= \frac{1}{\pi a^3} \int \exp\left(-\frac{2r'}{a}\right) \exp(i\mathbf{q}\cdot\mathbf{r}') d\mathbf{r}' \\ &= \frac{4}{a^3} \int_0^\infty \exp\left(-\frac{2r'}{a}\right) \frac{\sin qr'}{qr'} r'^2 dr', \end{aligned} \tag{5.10}$$

which is a function of q^2 only:

$$F_e(q^2) = \left[1 + \left(\frac{aq}{2}\right)^2\right]^{-2}. \tag{5.11}$$

In the next section we shall derive an expression for the form factor when we use harmonic oscillator functions to describe the ground state of the hydrogen atom. We shall then compare the results for different number of quanta in the approximation with the exact result.

6 Theoretical Form Factor of the Hydrogen Atom Using Harmonic Oscillator States

Suppose we do not know the exact wave function for the ground state of the hydrogen atom but that we could approximate it in terms of harmonic oscillator functions for up to $\mathfrak{N}$ quanta, *i.e.*,

$$\psi = \sum_n a_n |n00\rangle = \frac{1}{\sqrt{(4\pi)}} \sum_n a_n R_{n0}(r), \quad n = 0, 1, \ldots, \tfrac{1}{2}\mathfrak{N}. \tag{6.1}$$

In this equation r is the dimensionless one of section 1. The coefficients a_n can be determined from the variational analysis discussed in (3.7), which leads to the following set of linear equations for a_n:

$$\sum_n \left\langle n'00 \left| \tfrac{1}{2}\epsilon^2 p^2 - \frac{\sqrt{2}\epsilon}{r} \right| n00 \right\rangle a_n = E(\epsilon) a_{n'}. \tag{6.2}$$

Here $E(\epsilon)$, the lowest eigenvalue for the matrix of the Hamiltonian in (6.2), is the function of ϵ plotted in Fig. I.1. If we take for ϵ the value that gives the minimum of $E(\epsilon)$ for $\mathfrak{N} = 0, 2, 4, 6, 8$ or 10 quanta, we can obtain the corresponding a_n for these cases.

The charge density associated with the ψ of (6.1) is given by

$$\rho(r) = \frac{1}{4\pi} \sum_{nn'} a^*_{n'} a_n R_{n'0}(r) R_{n0}(r), \tag{6.3}$$

and so the corresponding form factor is, from (5.8),

$$F(q^2) = \int \exp(i\kappa \cdot \mathbf{r})\rho(\mathbf{r})d\mathbf{r}$$
$$= 4\pi \int_0^\infty \rho(r)\frac{\sin \kappa r}{\kappa r} r^2 dr = \sum_{n'n} a^*_{n'} a_n M_{n'n}(\kappa^2). \tag{6.4}$$

In (6.4) κ^2 is related to q^2 by

$$\kappa^2 = \frac{\hbar}{m\omega} q^2 = 2\left(\frac{\hbar^2}{me^2}\right)^2 \frac{1}{\epsilon^2} q^2, \tag{6.5}$$

as the $\mathbf{r}$ in the integral is dimensionless. Furthermore,

$$M_{n'n}(\kappa^2) \equiv \int_0^\infty R_{n'0}(r)\frac{\sin \kappa r}{\kappa r} R_{n0}(r) r^2 dr = \sum_{p=o}^{n'+n} B(n'0, n0, p) I_p(\kappa^2), \tag{6.6}$$

with

$$I_p(\kappa^2) = \frac{2}{\Gamma(p+\frac{3}{2})} \int_0^\infty r^{2p+2} \frac{\sin \kappa r}{\kappa r} e^{-r^2} dr$$
$$= \tfrac{1}{2} e^{-\kappa^2/4} \sum_{s=0}^{p} \binom{2p+1}{2s} \frac{\Gamma(s+\frac{1}{2})}{\Gamma(p+\frac{3}{2})} \left(-\frac{\kappa^2}{4}\right)^{p-s}, \tag{6.7}$$

as can be easily seen by integration by parts.

Using for a_n the values obtained by this variational procedure for $\mathfrak{N} = 0, 4$ and 8 and taking the appropriate value of ϵ in (6.5) for these three cases, Yeh [12] computed the corresponding form factors; they are plotted in Fig. I.3, where he also plotted the exact form factor $F_e(q^2)$. Note that the curves are plotted in a semilogarithmic scale, so that in the zero-quantum approximation we get just a straight line. From the figure we see clearly that we can approach the exact form factor as closely as we want if we increase the number of quanta $\mathfrak{N}$ in the analysis.

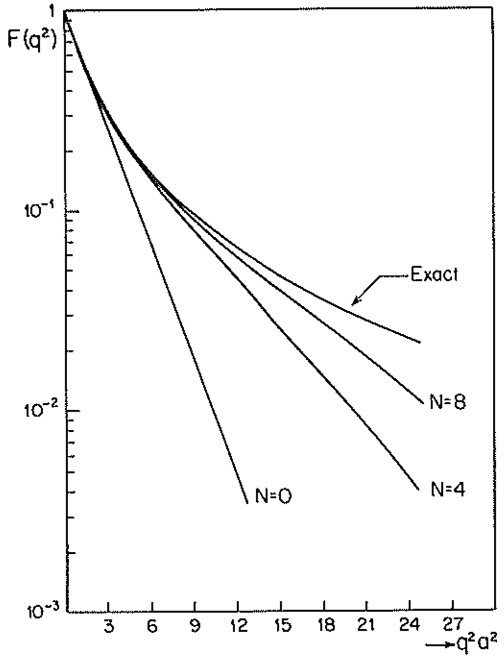

Figure I.3. Form factor for the electronic charge of the ground state of the H atom as a function of the square of the momentum transfer q^2. The upper line is the exact form factor (5.11). The other lines are the form factors (6.4) for the linear combination of harmonic-oscillator states obtained by the variational analysis of §3. The notation $N = 0, 4, 8$ stands for the maximum number of quanta in the expansion.

In Fig. I.3 we included only the form factor for expansions of ψ that differ by jumps of four quanta, for the reasons stressed at the end of section 3.

In the next section we discuss an alternative procedure for getting the a_n directly from the experiment, or in the case of the hydrogen atom the exact, form factor, thus bypassing the variational analysis of this section which requires the knowledge of the Hamiltonian in (6.2).

7 Direct Determination of the Ground State Through a Least-Squares Approach to the Form Factor. The Pseudo Hartree–Fock (PHF) Approximation

Suppose that we do not know the potential in the hydrogen atom but that we have at our disposal the experimental data for the form factor taken from the elastic scattering of electrons by hydrogen atoms. These experimental results will be assumed here to be the same as Eq. (5.11), *i.e.*, $F_e(q^2) = [1+(qa/2)^2]^{-2}$, since this is the exact form factor.

Consider now the derivative of $F_e(q^2)$ with respect to q^2 computed at the point $q^2 = 0$. This gives us the slope of $F_e(q^2)$ at $q^2 = 0$. We shall show that this slope is proportional to the mean square radius and later use this result to fix the frequency of the harmonic oscillator states we require. To obtain the derivative dF/dq^2 we see from Eq. (6.4) that essentially we have to calculate

$$\frac{d}{dq^2}\frac{\sin qr'}{qr'} = \frac{1}{2q}\frac{d}{dq}\frac{\sin qr'}{qr'} = \frac{1}{2q^2}\left(\cos qr' - \frac{\sin qr'}{qr'}\right). \tag{7.1}$$

Expanding $\cos qr'$ and $\sin qr'/qr'$ in power series we get finally

$$\left[\frac{d}{dq^2}\frac{\sin qr'}{qr'}\right]_{q^2=0} = -\frac{1}{6}r'^2, \tag{7.2}$$

so that

$$\left(\frac{dF}{dq^2}\right)_{q^2=0} = -\frac{4\pi}{6}\int_0^\infty \rho(r')r'^4 dr'. \tag{7.3}$$

Now the $\rho(r')$ associated with $F_e(q^2)$ is $(\pi a^3)^{-1}\exp(-2r'/a)$ so that

$$\left(\frac{dF_e}{dq^2}\right)_{q^2=0} = -\tfrac{1}{2}a^2. \tag{7.4}$$

Note that this result could be obtained directly from (5.11); however, Eq. (7.3) holds for the $\rho(r')$ associated with any wave function describing the ground state of the hydrogen atom. We shall use it with the harmonic oscillator expression (6.1) and then compare with (7.4). In this way we shall fix ϵ.

With a harmonic oscillator of zero quanta we get

$$\rho(r) = \pi^{-\frac{3}{2}}e^{-r^2}, \tag{7.5}$$

where now r is the dimensionless variable of section 1. Putting this $\rho(r)$ into Eq. (7.3) we obtain

$$\left(\frac{dF}{dq^2}\right)_0 = \frac{\hbar}{m\omega}\left(\frac{dF}{d\kappa^2}\right)_0 = \frac{\hbar}{m\omega}\left[-\frac{4\pi}{6}\int_0^\infty r^4\pi^{-\frac{3}{2}}e^{-r^2}dr\right] = -\frac{1}{4}\frac{\hbar}{m\omega}, \tag{7.6}$$

where we have used the relation between κ^2 and q^2 of (6.5) which is needed for the dimensionless r. Equating this result with the "experimental" value of Eq. (7.4), we have

$$\frac{1}{4}\frac{\hbar}{m\omega} = \frac{1}{2}a^2 = \frac{1}{2}\frac{\hbar^4}{m^2e^4}, \tag{7.7}$$

or

$$\frac{\hbar\omega}{(me^4/2\hbar^2)} = \epsilon = 1. \tag{7.8}$$

Thus from the form factor we have determined the value 1 for our parameter ϵ. This is in good agreement with the variational analysis in the zero-quantum approximation, where we get $\epsilon = 1.06$ [see Eq. (3.13)].

To define completely the wave function of Eq. (6.1) there remains the problem of determining the coefficients a_n. We shall do this by a least-squares fitting of the $F(q^2)$ of (6.4) to the $F_e(q^2)$ subject to the constraint that ψ is normalized; *i.e.*, we shall minimize the expression

$$\int_0^\infty [F(q^2) - F_e(q^2)]^2 dq^2 - \lambda\sum_n a_n^* a_n, \quad n = 0, 1, \ldots, \tfrac{1}{2}\mathfrak{N}, \tag{7.9}$$

where λ is a Lagrange multiplier. From (6.4) this expression becomes

$$\begin{aligned}\sum_{\substack{n'n\\m'm}} a_{n'}^* a_{m'}^* a_n a_m \int_0^\infty M_{n'n}(q^2)M_{m'm}(q^2)dq^2 \\ -2\sum_{n'n} a_{n'}^* a_n \int_0^\infty M_{n'n}(q^2)F_e(q^2)dq^2 \\ +\int_0^\infty [F_e(q^2)]^2dq^2 - \lambda\sum_{n'n} a_{n'}^* a_n \delta_{n'n}.\end{aligned} \tag{7.10}$$

All sums go from 0 to $\frac{1}{2}\mathfrak{N}$, and $M_{n'n}(q^2)$ are given by (6.6), so that taking its derivative with respect to a_k^* we obtain the following system of algebraic equations:

$$2\sum_n\left[\sum_{m'm}a^*_{m'}a_m\int_0^\infty M_{kn}(q^2)M_{m'm}(q^2)dq^2\right]a_n$$
$$-2\sum_n\left[\int_0^\infty M_{kn}(q^2)F_e(q^2)dq^2\right]a_n=\lambda a_k. \tag{7.11}$$

We solve (7.11) by successive approximations. Starting with a first guess $a_n^{(0)}$, we use (6.4) to define, from the $(p-1)th$ approximation $a_n^{(p-1)}$, the quantity

$$F^{(p-1)}(q^2)\equiv\sum_{m'm}a^{*(p-1)}_{m'}a^{(p-1)}_m M_{m'm}(q^2). \tag{7.12}$$

Substituting in (7.11), we obtain a set of equations which is linear:

$$2\sum_n\left[\int_0^\infty dq^2[F^{(p-1)}(q^2)-F_e(q^2)]M_{kn}(q^2)\right]a_n^{(p)}=\lambda a_k^{(p)}. \tag{7.13}$$

We continue this process until (7.13) has a self-consistent solution, *i.e.*, until $a_n^{(p)}=a_n^{(p-1)}$ to the approximation desired.

Equations (7.11) and the method we propose for solving them are very similar to those used in the Hartree–Fock approximation [13], which is why we shall refer to this procedure of getting the coefficients a_n, as the Pseudo Hartree–Fock (PHF) approximation.

Equations (7.13) were solved by A.M. Cetto [14] for $\mathfrak{N}=2$ and $\epsilon=1$; she obtained the following results:

$$\begin{array}{lll} a_0^{(0)}=1 & a_0^{(1)}=0.680 & a_0^{(2)}=0.650 \\ a_1^{(0)}=0 & a_1^{(1)}=0.733 & a_1^{(2)}=0.760 \end{array} \tag{7.14}$$

Thus self-consistency was practically achieved after two steps [14].

8 The One-Body Harmonic Oscillator States Expressed in Terms of Creation Operators

If we have a one-dimensional harmonic oscillator we know that the states are characterized by an integer quantum number n and can be expressed in terms of a creation operator applied to the ground state in the following way:

$$|n\rangle=\frac{1}{\sqrt{n!}}\eta^n|0\rangle,\quad |0\rangle=\pi^{-\frac14}e^{-\frac12x^2}, \tag{8.1}$$

where

$$\eta=\frac{1}{\sqrt2}(x-ip)=\frac{1}{\sqrt2}\left(x-\frac{d}{dx}\right). \tag{8.2}$$

It is easy to prove that $|n\rangle$ is an eigenstate of H:

$$H|n\rangle=\tfrac12(p^2+x^2)|n\rangle=(n+\tfrac12)|n\rangle. \tag{8.3}$$

In order to see this, define the annihilation operator

$$\xi=\eta^\dagger=\frac{1}{\sqrt2}(x+ip)=\frac{1}{\sqrt2}\left(x+\frac{d}{dx}\right), \tag{8.4}$$

so that from (8.1) we obtain

$$\xi|0\rangle=\frac{1}{\sqrt2}\left(x+\frac{d}{dx}\right)\pi^{-\frac14}e^{-\frac12x^2}=\frac{\pi^{-\frac14}}{\sqrt2}x[e^{-\frac12x^2}-e^{-\frac12x^2}]=0. \tag{8.5}$$

On the other hand we have the commutator $[\xi,\eta]=1$, so that

$$H|n\rangle=\tfrac12(p^2+x^2)|n\rangle=(\eta\xi+\tfrac12)|n\rangle=\eta\xi\frac{1}{\sqrt{n!}}\eta^n|0\rangle+\tfrac12|n\rangle$$
$$=\frac{1}{\sqrt{n!}}\eta[\xi,\eta^n]|0\rangle+\tfrac12|n\rangle=\frac{n}{\sqrt{n!}}\eta^n|0\rangle+\tfrac12|n\rangle=(n+\tfrac12)|n\rangle, \tag{8.6}$$

where we have used the result $[\xi,\eta^n]=n\eta^{n-1}$.

The generalization for three dimensions is immediate. In this case the functions are given by

$$|n_1n_2n_3\rangle=[n_1!n_2!n_3!]^{-\frac12}\eta_1^{n_1}\eta_2^{n_2}\eta_3^{n_3}|0\rangle, \tag{8.7}$$

with

$$\eta_j=\frac{1}{\sqrt2}(x_j-ip_j),\ \xi_j=\eta_j^\dagger,\ j=1,2,3. \tag{8.8}$$

Now the normalized ground state is described by

$$|0\rangle=\pi^{-\frac34}\exp[-\frac12(x_1^2+x_2^2+x_3^2)]. \tag{8.9}$$

In these coordinates (Cartesian) the quantum numbers are n_1,n_2 and n_3, associated with the integrals of motion H_1,H_2 and H_3. The states (8.7) in general are not eigenstates of L^2 or L_3. If we want to characterize the to obtain appropriate homogeneous polynomials of degree N in the $\eta_i' s$. To derive them we first discuss the following auxiliary problem: What is the polynomial $P = P(x_1, x_2, x_3)$ that satisfies the equations

$$\left.\begin{array}{rcl} \mathbf{r}\cdot\nabla P &=& NP \\ \mathbf{L}^2 P &=& l(l+1)P \\ L_3 P &=& mP \end{array}\right\}, \tag{8.10}$$

with N, l, m integers, $-l \leq m \leq l, N \geq l$ and $N - l$ even? Clearly it is the homogeneous polynomials of degree $N, r^N Y_{lm}(\theta, \varphi)$, where Y_{lm} is the usual spherical harmonic. Introducing the concept of solid spherical harmonic

$$\mathcal{Y}_{lm}(\mathbf{x}) \equiv r^l Y_{lm}(\theta, \varphi), \tag{8.11}$$

the solution could also be written as

$$(\mathbf{x}\cdot\mathbf{x})^n \mathcal{Y}_{lm}(\mathbf{x}), \qquad \text{with} \qquad N = 2n + l. \tag{8.12}$$

Let us now return to the creation and annihilation operators η_i, ξ_j. From (8.8) it is easy to see that

$$[\xi_i, \eta_j] = \delta_{ij}, \quad [\xi_i, \xi_j] = [\eta_i, \eta_j] = 0, \tag{8.13}$$

and

$$\boldsymbol{\eta}\times\boldsymbol{\xi} = \tfrac{1}{2} i(\mathbf{x}\times\mathbf{p} - \mathbf{p}\times\mathbf{x}) = i\mathbf{x}\times\mathbf{p}, \tag{8.14}$$

so that

$$\mathbf{L} = -i\boldsymbol{\eta}\times\boldsymbol{\xi}. \tag{8.15}$$

From (8.13) we conclude that ξ_j, when acting on a polynomial in the creation operators η_j can be interpreted as the operator $\partial/\partial\eta_j$, for the same reasons that $p = -i\partial/\partial x_j$. It is clear therefore from (8.10) and (8.12) that the state

$$|nlm\rangle \equiv A_{nl}(\boldsymbol{\eta}\cdot\boldsymbol{\eta})^n \mathcal{Y}_{lm}(\boldsymbol{\eta})|0\rangle, \tag{8.16}$$

in which A_{nl} is a normalization constant, satisfies the equations

$$\left.\begin{array}{l} (H - \frac{3}{2})|nlm\rangle = \boldsymbol{\eta}\cdot\boldsymbol{\xi}|nlm\rangle = N|nlm\rangle \\ L^2|nlm\rangle = l(l+1)|nlm\rangle \\ L_3|nlm\rangle = m|nlm\rangle \end{array}\right\}. \tag{8.17}$$

Thus $|nlm\rangle$, defined by (8.16), is simultaneously an eigenfunction of H, L^2, L_3, and is given in terms of a definite homogeneous polynomial of degree $N = 2n + l$ in the η_j applied to the ground state:

$$|0\rangle \equiv \pi^{-\frac{3}{4}} e^{-\frac{1}{2}r^2}. \tag{8.18}$$

The normalization coefficient A_{nl}, derived in the next section, is

$$A_{nl} = (-1)^n \left[\frac{4\pi}{(2n + 2l + 1)!!(2n)!!}\right]^{\frac{1}{2}}. \tag{8.19}$$

9 Normalization Coefficients of the Harmonic Oscillator States

The normalization constant A_{nlm} may be calculated by computing the scalar product of $|nlm\rangle$ with itself:

$$1 = \langle nlm|nlm\rangle = |A_{nlm}|^2 \langle 0|\mathcal{Y}^\dagger_{lm}(\boldsymbol{\eta})(\boldsymbol{\xi}\cdot\boldsymbol{\xi})^n(\boldsymbol{\eta}\cdot\boldsymbol{\eta})^n \mathcal{Y}_{lm}(\boldsymbol{\eta})|0\rangle. \tag{9.1}$$

The first step is to develop a recursion relation in n which enables us to relate this matrix element to that for $n = 0$, which may then be easily evaluated. From the correspondence $\xi_j \rightarrow \partial/\partial\eta_j$ we see that $\boldsymbol{\xi}\cdot\boldsymbol{\xi}$ will operate on $(\boldsymbol{\eta}\cdot\boldsymbol{\eta})^n\mathcal{Y}_{lm}(\boldsymbol{\eta})$ in the same way as the Laplacian

$$\nabla^2 = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) - \frac{L^2}{r^2} \tag{9.2}$$

does on $(\mathbf{x}\cdot\mathbf{x})^n\mathcal{Y}_{lm}(\mathbf{r})$; this is found easily:

$$\begin{aligned} \nabla^2(\mathbf{x}\cdot\mathbf{x})^n\mathcal{Y}_{lm}(\mathbf{r}) &= \nabla^2 r^{2n+l} Y_{lm}(\theta, \varphi) \\ &= [(2n + l)(2n + l + 1) - l(l + 1)]r^{2n-2}\mathcal{Y}_{lm}(\mathbf{r}) \\ &= 2n(2n + 2l + 1)r^{2n-2}\mathcal{Y}_{lm}(\mathbf{r}). \end{aligned} \tag{9.3}$$

Using this analogy, the scalar product (9.1) becomes

$$\begin{aligned} &\langle 0|\mathcal{Y}^\dagger_{lm}(\boldsymbol{\eta})(\boldsymbol{\xi}\cdot\boldsymbol{\xi})^n(\boldsymbol{\eta}\cdot\boldsymbol{\eta})^n\mathcal{Y}_{lm}(\boldsymbol{\eta})|0\rangle \\ &\quad = 2n(2n + 2l + 1)\langle 0|\mathcal{Y}^\dagger_{lm}(\boldsymbol{\eta})(\boldsymbol{\xi}\cdot\boldsymbol{\xi})^{n-1}(\boldsymbol{\eta}\cdot\boldsymbol{\eta})^{n-1}\mathcal{Y}_{lm}(\boldsymbol{\eta})|0\rangle \\ &\quad = \frac{(2n)!!(2n + 2l + 1)!!}{(2l + 1)!!}\langle 0|\mathcal{Y}^\dagger_{lm}(\boldsymbol{\eta})\mathcal{Y}_{lm}(\boldsymbol{\eta})|0\rangle. \end{aligned} \tag{9.4}$$

The analysis is now simplified by noting that the scalar product in (9.4) is independent of m. This can be seen as follows: recall that

$$L_+|0lm\rangle = [(l - m)(l + m + 1)]^{\frac{1}{2}}|0lm + 1\rangle \tag{9.5}$$

or

$$[(l-m)(l+m+1)]^{-\frac{1}{2}}L_+|0lm\rangle = |0lm+1\rangle. \tag{9.6}$$

Thus, we have

$$\langle 0|\mathcal{Y}^\dagger_{lm+1}\mathcal{Y}_{lm+1}|0\rangle = [(l-m)(l+m+1)]^{-1}\langle 0|\mathcal{Y}^\dagger_{lm}L_-L_+\mathcal{Y}_{lm}|0\rangle. \tag{9.7}$$

Using $L^2 = L_-L_+ + L_0(L_0+1)$, we obtain

$$\langle 0|\mathcal{Y}^\dagger_{lm+1}\mathcal{Y}_{lm+1}|0\rangle = \frac{l(l+1)-m(m+1)}{(l-m)(l+m+1)}\langle 0|\mathcal{Y}^\dagger_{lm}\mathcal{Y}_{lm}|0\rangle = \langle 0|\mathcal{Y}^\dagger_{lm}\mathcal{Y}_{lm}|0\rangle, \tag{9.8}$$

which is the desired result. We may now drop the m index on A_{nlm}, as was already done in (8.16).

Thus we may choose, without loss of generality $m = l$; $\mathcal{Y}_{lm}(\mathbf{x})$ then reduces to [15]

$$\begin{aligned}\mathcal{Y}_{ll}(\mathbf{r}) &= (-)^l\sqrt{\left(\frac{(2l+1)!}{2}\right)}\frac{r^l}{l!2^l}\sin^l\theta\frac{1}{\sqrt{(2\pi)}}e^{il\varphi}\\ &= \sqrt{\left(\frac{(2l+1)!}{2^l4\pi}\right)}\frac{1}{l!}(x_+)^l,\end{aligned} \tag{9.9}$$

where

$$x_\pm \equiv \mp\frac{1}{\sqrt{2}}(x_1 \pm ix_2). \tag{9.10}$$

In analogy we have

$$\mathcal{Y}_{ll}(\eta) = \sqrt{\left(\frac{(2l+1)!}{2^l4\pi}\right)}\frac{1}{l!}(\eta_+)^l, \tag{9.11}$$

where

$$\eta_\pm = \mp\frac{1}{\sqrt{2}}(\eta_1 \pm i\eta_2). \tag{9.12}$$

Then,

$$\langle 0|\mathcal{Y}^\dagger_{ll}(\eta)\mathcal{Y}_{ll}(\eta)|0\rangle = \frac{(2l+1)!}{4\pi}\frac{1}{2^l(l!)^2}\langle 0|(\eta^\dagger_+)^l(\eta_+)^l|0\rangle = \frac{(2l+1)!!}{4\pi}. \tag{9.13}$$

Using (9.4) and (9.13), (9.1) becomes

$$\langle nlm|nlm\rangle = |A_{nl}|^2\frac{(2n)!!(2n+2l+1)!!}{(2l+1)!!}\frac{(2l+1)!!}{4\pi}, \tag{9.14}$$

or

$$A_{nl} = e^{i\delta_{nl}}\left[\frac{4\pi}{(2n)!!(2n+2l+1)!!}\right]^{\frac{1}{2}}. \tag{9.15}$$

We shall choose the phase factor $e^{i\delta_{nl}}$ to conform with the standard definition of the associated Laguerre polynomial [16] in which the coefficient a_{nl0} of (1.8) is positive.

From (1.8) and (9.9) we see that

$$|nll\rangle = \sqrt{\left(\frac{(2l+1)!}{2^l4\pi}\right)}\frac{1}{l!}x^l_+\sum_{k=0}^{n}a_{nlk}r^{2k}e^{-\frac{1}{2}r^2}, \tag{9.16}$$

with a_{nlk} given by (1.9), while in terms of creation operators $|nll\rangle$ is given by

$$|nll\rangle = A_{nl}\sqrt{\left(\frac{(2l+1)!}{2^l4\pi}\right)}\frac{1}{l!}(\eta\cdot\eta)^n\eta^l_+|0\rangle. \tag{9.17}$$

To compare the two so as to get the phase factor we first note that

$$\eta_+ = \frac{1}{\sqrt{2}}(x_+ - ip_+) = \frac{1}{\sqrt{2}}\left(x_+ - \frac{\partial}{\partial x^+}\right) = \frac{1}{\sqrt{2}}\left(x_+ + \frac{\partial}{\partial x_-}\right), \tag{9.18}$$

then we use (9.16), (9.17) and the fact that $r^2 = -2x_+x_- + x_0^2$ so that $\partial f(r)/\partial x_- = -(x_+/r)\partial f/\partial r$; therefore we get

$$\left.\begin{aligned}|nl+1l+1\rangle &= \frac{A_{nl+1}}{A_{nl}}\left[\frac{(2l+3)(2l+2)}{2}\right]^{\frac{1}{2}}\frac{1}{l+1}\eta_+|nll\rangle\\ &= \frac{A_{nl+1}}{A_{nl}}\frac{[(2l+3)(2l+2)]^{\frac{1}{2}}}{2(l+1)}\left(x_+ + \frac{\partial}{\partial x_-}\right)|nll\rangle\\ &= \frac{A_{nl+1}}{A_{nl}}\left[\frac{(2l+3)!}{4\pi 2^l}\right]^{1/2}\frac{1}{(l+1)!}\sum_k\left[a_{nlk} - (k+1)a_{nlk+1}\right]r^{2k}e^{-\frac{1}{2}r^2}x^l_+\end{aligned}\right\}. \tag{9.19}$$

Thus we obtain

$$a_{nl+10} = \frac{A_{nl+1}}{A_{nl}}\sqrt{2}(a_{nl0} - a_{nl1}), \tag{9.20}$$

where because of (1.9) the bracket is positive, implying that A_{nl+1} and A_{nl} have the same sign. As the reasoning can be repeated when we apply powers of the operator η_+, it is clear that the phase factor is independent of l.

We now note that

$$\boldsymbol{\eta} \cdot \boldsymbol{\eta} = r^2 - \tfrac{1}{2}(p^2 + r^2) - \tfrac{3}{2} - i\mathbf{r} \cdot \mathbf{p} = r^2 - H_{\text{ho}} - \tfrac{3}{2} - \mathbf{r} \cdot \nabla, \qquad (9.21)$$

so from (9.16) and (9.17) we get

$$\begin{aligned} |n+1ll) &= \frac{A_{n+1l}}{A_{nl}}(\boldsymbol{\eta} \cdot \boldsymbol{\eta})|nll) \\ &= \frac{A_{n+1l}}{A_{nl}} \sqrt{\left(\frac{(2l+1)!}{2^l 4\pi}\right)} \frac{1}{l!} \left(\frac{x_+}{r}\right)^l \\ &\quad \sum_k [2a_{nlk-1} - (2n+2k+l+3)a_{nlk}] r^{2k+l} e^{-\frac{1}{2}r^2}. \end{aligned} \qquad (9.22)$$

Thus we obtain

$$a_{n+1l0} = -\frac{A_{n+1l}}{A_{nl}}(2n+l+3)a_{nl0}, \qquad (9.23)$$

implying that A_{n+1l} and A_{nl} have opposite sign.

Since by definition $A_{00} = 1$, we see from the above discussion that the phase factor in (9.15) becomes

$$e^{i\delta_{nl}} = (-1)^n. \qquad (9.24)$$

This is the phase factor of (8.19).

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