Quantum Mechanics: Chapter 4 Problems

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Problem 4.47

Solve 3D QHO using seperation of variables in Spherical Coordinates (as the potential is spherically symmetrical). Find the recursion formulas and determine the allowed energies.

$$\psi(r,\theta,\phi) = R(r)Y(\theta,\phi) \tag{1}$$

where

$$Y(\theta,\phi) = \sqrt{\frac{(2l+1)}{4\pi}\frac{(l-m)!}{(l+m)!}}e^{im\phi}P_l^m(\cos(\theta)) \tag{2}$$

The Radial Equation is

$$-\frac{\hbar^2}{2m}\frac{d^2u}{dr^2} + \left[V + \frac{\hbar^2}{2m}\frac{l(l+1)}{r^2}\right]u = Eu$$

since $V(r) = \frac{m\omega^2 r^2}{2}$,

$$-\frac{\hbar^2}{2m}\frac{d^2u}{dr^2} + \left[\frac{m\omega^2 r^2}{2} + \frac{\hbar^2}{2m}\frac{l(l+1)}{r^2}\right]u = Eu$$

define $\xi \equiv \sqrt{\frac{m\omega}{\hbar}}r$ and then $\frac{d^2u}{dr^2}$ becomes $\frac{m\omega}{\hbar}\frac{d^2u}{d\xi^2}$.

$$-\frac{\hbar^2}{2m}\frac{m\omega}{\hbar}\frac{d^2u}{d\xi^2} + \left[\frac{m\omega^2 r^2}{2}\frac{\hbar}{m\omega r^2}\xi^2 + \frac{\hbar^2}{2m}\frac{l(l+1)}{r^2}\right]u = Eu$$

multiply by $\frac{2}{\hbar\omega}$ on both sides and transpose the effective potential to the right side.

$$\frac{d^2u}{d\xi^2} = \left[\xi^2 + \frac{\hbar}{m\omega}\frac{l(l+1)}{r^2} - \frac{2E}{\hbar\omega}\right]u$$

define $K \equiv \frac{2E}{\hbar\omega}$

$$\frac{d^2u}{d\xi^2} = \left[\xi^2 + \frac{l(l+1)}{\xi^2} - K\right]u \tag{3}$$

To get an approximate solution, For $\xi >> 1$

$$\frac{d^2u}{d\xi^2} \approx \xi^2 u$$

$$\implies u(\xi) \approx Ae^{\frac{-\xi^2}{2}} + Be^{\frac{\xi^2}{2}} \implies u(\xi) \approx Ae^{\frac{-\xi^2}{2}} \text{(B=0 otherwise the equation will blow up)}$$

For $\xi << 1$,

$$\frac{d^2u}{d\xi^2} \approx \frac{l(l+1)}{\xi^2}u$$

$$\implies u(\xi) \approx C\xi^{l+1} + D\xi^{-l} \implies u(\xi) \approx C\xi^{l+1} \text{(D=0 otherwise } 1/\xi^l \to \infty)$$

$\therefore u(\xi) = \xi^{l+1}e^{\frac{-\xi^2}{2}}v(\xi)$. hopefully, $v(\xi)$ will turn out to be simpler than $u(\xi)$.

$$
\begin{aligned}
\frac{du}{d\xi} &= (\xi^{l+1})'(e^{\frac{-\xi^2}{2}}v(\xi)) + (\xi^{l+1})(e^{\frac{-\xi^2}{2}}v(\xi))' \\
&= ((l+1)\xi^l)(e^{\frac{-\xi^2}{2}}v(\xi)(\xi)) + (\xi^{l+1})(-\xi e^{\frac{-\xi^2}{2}}v(\xi) + \frac{dv}{d\xi}e^{\frac{-\xi^2}{2}}) \\
&= (l+1)\xi^l e^{\frac{-\xi^2}{2}}v + \xi^{l+1}e^{\frac{-\xi^2}{2}}v' - \xi^{l+2}e^{\frac{-\xi^2}{2}}v \qquad (4)
\end{aligned}
$$

and

$$
\begin{aligned}
\frac{d^2u}{d\xi^2} &= -2(l+3)\xi^{l+1}e^{\frac{-\xi^2}{2}}v + 2(l+1)\xi^l e^{\frac{-\xi^2}{2}}v' - 2\xi^{l+2}e^{\frac{-\xi^2}{2}}v' + \\
&\xi^{l+1}e^{\frac{-\xi^2}{2}}v'' - K\xi^{l+1}e^{\frac{-\xi^2}{2}}v \qquad (5)
\end{aligned}
$$

$\therefore$ Equation (3) becomes

$$
v'' + 2v'\left(\frac{l+1}{\xi} - \xi\right) + (K - 2l - 3)v = 0 \qquad (6)
$$

Let $v(\xi) \equiv \sum_{j=0}^{\infty} a_j\xi^j$ so, $v' = \sum_{j=1}^{\infty} ja_j\xi^{j-1} = \sum_{j=0}^{\infty} ja_j\xi^{j-1}$ and $\sum_{j=2}^{\infty} j(j-1)a_j\xi^{j-2}$

Substitute this to (6) and we get:

$$
\sum_{j=2}^{\infty} j(j-1)a_j\xi^{j-2} + 2(l+1)\sum_{j=1}^{\infty} ja_j\xi^{j-2} - \sum_{j=1}^{\infty} ja_j\xi^j + (K-2l-3)\sum_{j=0}^{\infty} a_j\xi^j = 0
$$

For the first two sums, make $j \to j+2$, note that $\sum_{j=1}^{\infty} ja_j\xi^{j-2} = a_1\xi^{-1} + \sum_{j=0}^{\infty}(j+2)a_{j+2}\xi^j$

$$
\sum_{j=0}^{\infty}(j+2)(j+1)a_{j+2}\xi^j + 2(l+1)\left(a_1\xi^{-1} + \sum_{j=0}^{\infty}(j+2)a_{j+2}\xi^j\right) - 2\sum_{j=0}^{\infty} ja_j\xi^j + (K-2l-3)\sum_{j=0}^{\infty} a_j\xi^j = 0
$$

Assuming $a_1 = 0$

$$
\sum_{j=0}^{\infty}[(j+2)(j+1)a_{j+2}\xi^j + 2(l+1)(j+2)a_{j+2}\xi^j - 2ja_j\xi^j + (K-2l-3)a_j\xi^j] = 0
$$

In order for the series to converge, ξ should have power 0

$$
\begin{aligned}
&= [(j+2)(j+2l+3)a_{j+2} + (K-2j-2l-3)a_j] = 0 \\
&= (j+2)(j+2l+3)a_{j+2} = (-K+2j+2l+3)a_j \\
&= \boxed{a_{j+2} = \frac{(2j+2l+3-K)}{(j+2)(j+2l+3)}a_j} \qquad (7)
\end{aligned}
$$

We have assumed $a_1 = 0$ so we get a sequence $a_0, a_2, etc.$ The sequence must terminate $\therefore \exists j_{max}$: $a_{j_{max}+2} = 0$

$$
\therefore 2j_{max} + 2l + 3 - K = 0
$$

since $K \equiv \frac{2E}{\hbar\omega}$

$$
E = \left(j_{max} + l + \frac{2}{3}\right)\hbar\omega
$$

Define $j_{max} + l \equiv n$

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