

3D simple harmonics using Ladder operator
Masatsugu Sei Suzuki
Department of Physics, SUNY at Binghamton
(Date: 2-02-15)

We discuss the quantum mechanics of three-dimensional simple harmonics by using the ladder operator method. This method is similar to that used for the derivation of wave function of hydrogen atom.

1. Ladder operator

The Hamiltonian of 3D simple harmonics is given in terms of the radial momentum p_r and the total orbital angular momentum L^2 as

$$\begin{aligned} H_l &= \frac{1}{2\mu} \left(p_r^2 + \frac{L^2}{r^2} \right) + \frac{1}{2} \mu \omega^2 r^2 \\ &= \frac{p_r^2}{2\mu} + \frac{l(l+1)\hbar^2}{2\mu r^2} + \frac{1}{2} \mu \omega^2 r^2 \quad , \\ &= \frac{\hbar^2}{2\mu} \left[\frac{p_r^2}{\hbar^2} + \frac{l(l+1)}{r^2} + \frac{\mu^2 \omega^2}{\hbar^2} r^2 \right] \end{aligned}$$

where the radial momentum operator p_r is given by

$$p_r = -i\hbar \frac{1}{r} \frac{\partial}{\partial r} r = -i\hbar \left(\frac{\partial}{\partial r} + \frac{1}{r} \right).$$

H_l is the Hamiltonian for a particle with mass μ that moves in one dimension in the effective potential

$$V_{eff}(r) = \frac{l(l+1)\hbar^2}{2\mu r^2} + \frac{1}{2} \mu \omega^2 r^2.$$

This potential can be rewritten as

$$V_{eff}(r) = V_{eff}(x) = \frac{\hbar\omega}{2} \left[\frac{l(l+1)}{x^2} + x^2 \right]$$

with

$$x = \frac{r}{\sqrt{\hbar/(\mu\omega)}}.$$

Here we make a plot of $V_{\text{eff}}(r)/(\hbar\omega/2)$ as a function of x , where $l = 0, 1, 2, 3, 4$, and 5

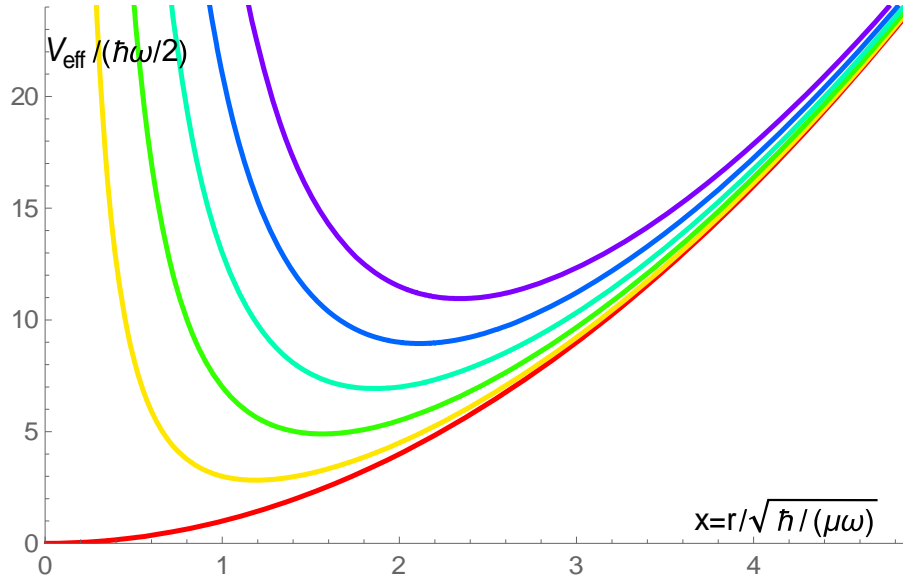


Fig. The effective potential for $l = 0 - 5$ [from bottom ($l = 0$, red) to top ($l = 5$, purple)]

Here we defined the ladder operator;

$$A_l = \frac{1}{\sqrt{2\mu\hbar\omega}} \left[ip_r - \frac{(l+1)\hbar}{r} + \mu\omega r \right],$$

The Hermite conjugate of A_l is

$$A_l^+ = \frac{1}{\sqrt{2\mu\hbar\omega}} \left[-ip_r - \frac{(l+1)\hbar}{r} + \mu\omega r \right]$$

We now calculate $A_l^+ A_l$

$$\begin{aligned}
A_l^+ A_l &= \frac{1}{2\mu\hbar\omega} \left[-ip_r - \frac{(l+1)\hbar}{r} + \mu\omega r \right] \left[ip_r - \frac{(l+1)\hbar}{r} + \mu\omega r \right] \\
&= \frac{1}{2\mu\hbar\omega} \left\{ p_r^2 + \left(-\frac{(l+1)\hbar}{r} + \mu\omega r \right)^2 + i \left[-\frac{(l+1)\hbar}{r} + \mu\omega r, p_r \right] \right\} \\
&= \frac{1}{2\mu\hbar\omega} \left\{ p_r^2 + \left(-\frac{(l+1)\hbar}{r} + \mu\omega r \right)^2 - i\mu\omega [p_r, r] + i \left[p_r, \frac{(l+1)\hbar}{r} \right] \right\} \\
&= \frac{1}{2\mu\hbar\omega} \left\{ p_r^2 + \left(-\frac{(l+1)\hbar}{r} + \mu\omega r \right)^2 - \mu\hbar\omega - \frac{(l+1)\hbar^2}{r^2} \right\} \\
&= \frac{1}{2\mu\hbar\omega} \left\{ p_r^2 + \frac{l(l+1)\hbar^2}{r^2} + \mu^2\omega^2 r^2 - \mu\hbar\omega(2l+3) \right\} \\
&= \frac{1}{\hbar\omega} H_l - \left(l + \frac{3}{2} \right)
\end{aligned}$$

Then we get

$$H_l = \hbar\omega \left\{ A_l^+ A_l + \left(l + \frac{3}{2} \right) \right\},$$

Here we note that

(i)

$$\begin{aligned}
\left[p_r, \frac{(l+1)}{r} \right] \psi(r) &= p_r \frac{l+1}{r} \psi - \frac{l+1}{r} p_r \psi \\
&= \frac{\hbar}{i} \frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{l+1}{r} \psi \right) - \frac{l+1}{r} \frac{\hbar}{i} \frac{1}{r} \frac{\partial}{\partial r} (r \psi) \\
&= \frac{\hbar}{i} \frac{(l+1)}{r} \frac{\partial}{\partial r} \psi - \frac{l+1}{r} \frac{\hbar}{i} \frac{1}{r} \left(\psi + r \frac{\partial}{\partial r} \psi \right) \\
&= -\frac{l+1}{r^2} \frac{\hbar}{i} \psi
\end{aligned}$$

(ii)

$$\begin{aligned}
[p_r, r]\psi(r) &= [p_r r \psi - r p_r \psi] \\
&= \frac{\hbar}{i} \frac{1}{r} \frac{\partial}{\partial r} (r^2 \psi) - r \frac{\hbar}{i} \frac{1}{r} \frac{\partial}{\partial r} (r \psi) \\
&= \frac{\hbar}{i} \frac{1}{r} (2r \psi + r^2 \frac{\partial}{\partial r} \psi) - \frac{\hbar}{i} (\psi + r \frac{\partial}{\partial r} \psi) \\
&= \frac{\hbar}{i} \psi
\end{aligned}$$

The commutation relation:

$$\begin{aligned}
[A_l, A_l^+] &= \frac{1}{2\mu\hbar\omega} [ip_r - \frac{(l+1)\hbar}{r} + \mu\omega r, -ip_r - \frac{(l+1)\hbar}{r} + \mu\omega r] \\
&= \frac{i}{\mu\hbar\omega} [p_r, -\frac{(l+1)\hbar}{r} + \mu\omega r] \\
&= \frac{i}{\mu\hbar\omega} \{-[p_r, \frac{(l+1)\hbar}{r}] + \mu\omega [p_r, r]\} \\
&= \frac{i}{\mu\hbar\omega} (\frac{l+1}{r^2} \frac{\hbar^2}{i} + \mu\omega \frac{\hbar}{i}) \\
&= 1 + \frac{(l+1)\hbar}{\mu\omega r^2}
\end{aligned}$$

or

$$[A_l, A_l^+] = \frac{H_{l+1} - H_l}{\hbar\omega} + 1,$$

since

$$H_{l+1} - H_l = \frac{\hbar^2}{2\mu r^2} [(l+2)(l+1) - l(l+1)] = \frac{\hbar^2}{\mu r^2} (l+1).$$

We also note that

$$H_l = \hbar\omega \{A_l^+ A_l + (l + \frac{3}{2})\}$$

and

$$\begin{aligned}[A_l, H_l] &= \hbar\omega[A_l, A_l^\dagger A_l] \\ &= \hbar\omega[A_l, A_l^\dagger]A_l \\ &= (H_{l+1} - H_l + \hbar\omega)A_l\end{aligned}$$

2. Eigenvalue problem

Suppose that $|E, l\rangle$ is an eigenket of H_l with eigenvalue E ,

$$H_l|E, l\rangle = E|E, l\rangle.$$

Then we get

$$\begin{aligned}A_l H_l |E, l\rangle &= A_l E |E, l\rangle \\ &= ([A_l, H_l] + H_l A_l) |E, l\rangle \\ &= (H_{l+1} + \hbar\omega) A_l |E, l\rangle\end{aligned}$$

or

$$H_{l+1} A_l |E, l\rangle = (E - \hbar\omega) A_l |E, l\rangle$$

This means that $A_l |E, l\rangle$ is the eigenket of H_{l+1} with the eigenvalue $E - \hbar\omega$. Then we have

$$A_l |E, l\rangle = \alpha_- |E - \hbar\omega, l+1\rangle.$$

where

$$H_{l+1} |E - \hbar\omega, l+1\rangle = (E - \hbar\omega) |E - \hbar\omega, l+1\rangle.$$

3. Eigenstates

A_l creates the radial wavefunction for a state has more orbital angular momentum and less energy than a state with which it started. In other words, A_l diminishes the radial

kinetic energy by some amount and adds a smaller quantity of energy to the tangential motion.

$$A_l |E, l\rangle \approx |E - \hbar\omega, l+1\rangle,$$

$$A_{l+1} |E - \hbar\omega, l+1\rangle \approx |E - 2\hbar\omega, l+2\rangle,$$

$$A_{l+2} |E - 2\hbar\omega, l+2\rangle \approx |E - 3\hbar\omega, l+3\rangle.$$

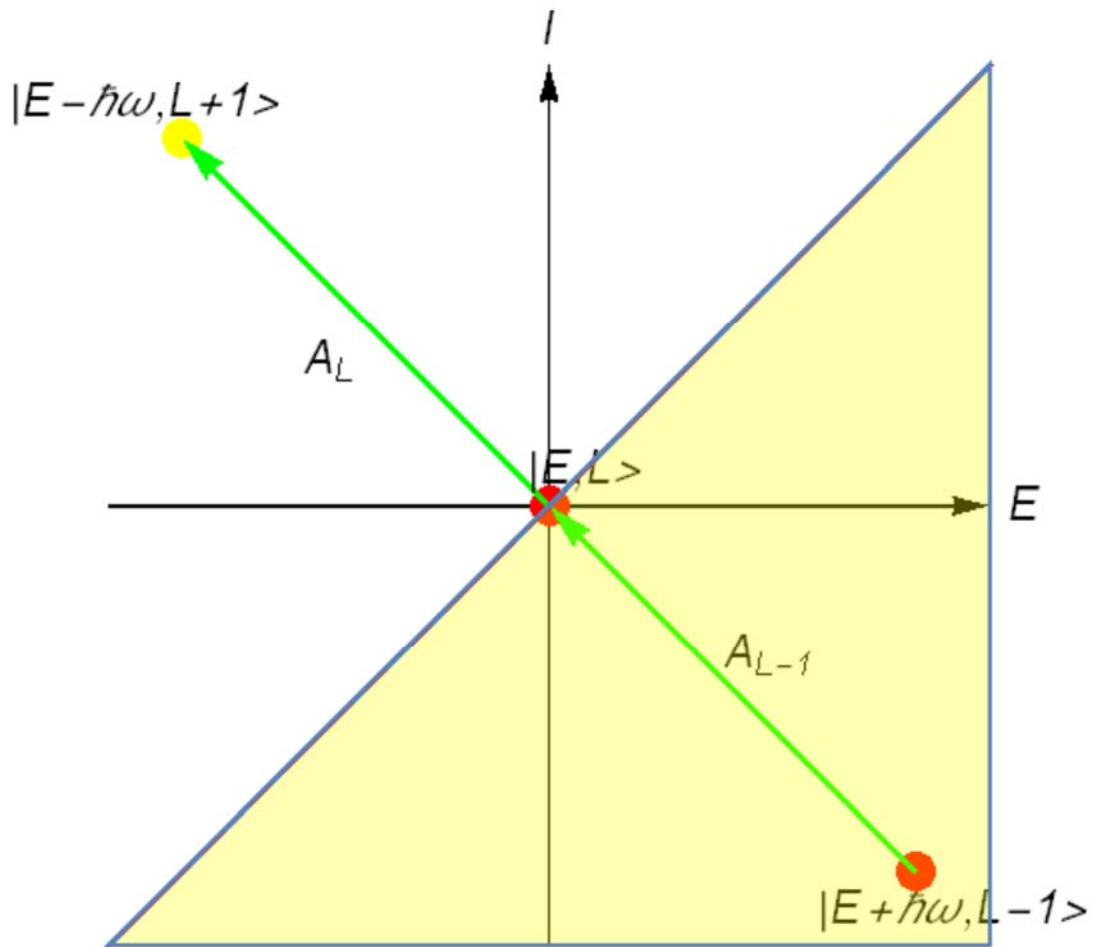


Fig. The boundary region [the allowed region below the straight line (purple line)] in the (E, l) plane with the action of A_l and A_{l-1} (denoted by green lines). The purple

lined is expressed by $E_L = \hbar\omega(L + \frac{3}{2})$. $A_L|E, L\rangle \approx |E - \hbar\omega, L+1\rangle = 0$.

$$H_L|E, L\rangle = E|E, L\rangle \quad . \quad A_{L-1}|E + \hbar\omega, L-1\rangle \approx |E, L\rangle \quad ,$$

$$H_{L-1}|E + \hbar\omega, L-1\rangle = E|E + \hbar\omega, L-1\rangle$$

Suppose that

$$A_L|E, L\rangle = 0 \quad (\text{a circuit orbit})$$

where L is the largest allowed value of l for energy E .

$$H_L|E_L, L\rangle = E_L|E_L, L\rangle = \hbar\omega(L + \frac{3}{2})|E_L, L\rangle .$$

where

$$H_L = \hbar\omega\{A_L^+ A_L + (L + \frac{3}{2})\} .$$

So we get

$$E_L = \hbar\omega(L + \frac{3}{2}) ,$$

where

$$L = 0, \quad E_L = \frac{3}{2}\hbar\omega ,$$

$$L = 1, \quad E_L = \frac{5}{2}\hbar\omega ,$$

$$L = 2, \quad E_L = \frac{7}{2}\hbar\omega ,$$

$$L = 3, \quad E_L = \frac{9}{2}\hbar\omega .$$

Since L is a non-negative integer, it follows that the ground state is $3\hbar\omega/2$ and that the ground state has no angular momentum. In general, $\frac{E}{\hbar\omega}$ is any integer plus $3/2$. These values of the allowed energies agree perfectly with what we could have deduced by treating H as a sum of 3D harmonic oscillator Hamiltonian.

4. A circuit orbit

$$A_L|E, L\rangle = 0$$

where

$$A_L = \frac{1}{\sqrt{2\mu\hbar\omega}} \left[ip_r - \frac{(L+1)\hbar}{r} + \mu\omega r \right]$$

$$\left(\frac{1}{r} \frac{\partial}{\partial r} r - \frac{L+1}{r} + \frac{\mu\omega}{\hbar} r \right) u_L(r) = 0$$

or

$$\left(\frac{\partial}{\partial r} - \frac{L}{r} + \frac{\mu\omega}{\hbar} r \right) u_L(r) = 0$$

where

$$\langle r | E, L \rangle = u_L(r),$$

$$l = \sqrt{\frac{\hbar}{2\mu\omega}}. \quad (\text{characteristic length for the simple harmonics})$$

We solve the first-order differential equation

$$\left(\frac{d}{dr} - \frac{L}{r} + \frac{1}{2l^2} r \right) u_L(r) = 0.$$

The solution of this differential equation:

$$\frac{du}{u} = \frac{L}{r} - \frac{1}{2l^2}r$$

$$\ln u = L \ln r - \frac{r^2}{4l^2}$$

$$u_L(r) = Cr^L \exp\left(-\frac{r^2}{4l^2}\right)$$

where C is the normalization constant. The radial probability density is

$$\begin{aligned} P(r, L)dr &= P(L, \xi)d\xi \\ &= r^2[u_L(r)]^2 dr \\ &= C^2 r^{2+2L} \exp\left(-\frac{r^2}{2l^2}\right) dr \\ &= \frac{1}{2^{L+\frac{1}{2}} \Gamma(L+\frac{3}{2})} l^{-(2L+3)} r^{2+2L} \exp\left(-\frac{r^2}{2l^2}\right) dr \\ &= \frac{1}{2^{L+\frac{1}{2}} \Gamma(L+\frac{3}{2})} \xi^{2+2L} \exp\left(-\frac{\xi^2}{2}\right) d\xi \end{aligned}$$

with

$$\xi = \frac{r}{l},$$

where

$$1 = \int_0^{\infty} dr r^2 [u_L(r)]^2 = C^2 \int_0^{\infty} r^{2+2L} \exp\left(-\frac{r^2}{2l^2}\right)$$

or

$$C = \frac{1}{\sqrt{2^{L+\frac{1}{2}} \Gamma(L+\frac{3}{2})}} l^{-(L+\frac{3}{2})}.$$

We make a plot of $P(L, \xi)$ as a function of $\xi = r/l$, where $L = 0, 1, 2, 3, \dots$,

$$P(L, \xi) = \frac{1}{2^{L+\frac{1}{2}} \Gamma(L+\frac{3}{2})} \xi^{2+2L} \exp\left(-\frac{\xi^2}{2}\right).$$

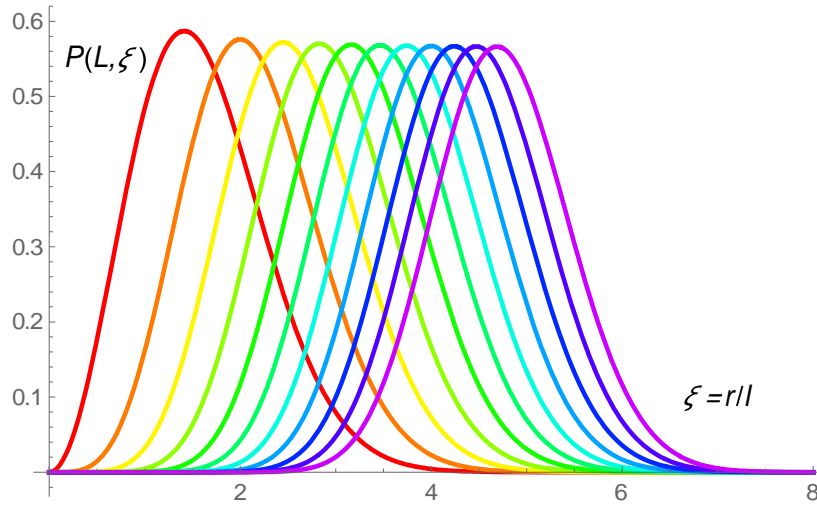


Fig. Radial probability distribution $P(L, \xi)$ of circular orbits in the 3D harmonic oscillator potential for $L = 0$ (red) into 10 (purple), as a function of $\xi = r/l$, with $l = \sqrt{\hbar/(2\mu\omega)}$.

This function has a peak at

$$\xi = \frac{r}{l} = \sqrt{2(L+1)}.$$

5. Degeneracy

$$A_l H_l = H_{l+1} A_l + \hbar\omega A_l,$$

$$H_l A_l^+ = A_l^+ H_{l+1} + \hbar\omega A_l^+,$$

$$H_{l+1} |E, l+1\rangle = E |E, l+1\rangle,$$

$$\begin{aligned} E A_l^+ |E, l+1\rangle &= A_l^+ H_{l+1} |E, l+1\rangle \\ &= (H_l A_l^+ - \hbar\omega A_l^+) |E, l+1\rangle \\ &= (H_l - \hbar\omega) A_l^+ |E, l+1\rangle \end{aligned}$$

or

$$H_l A_l^+ |E, l+1\rangle = (E + \hbar\omega) A_l^+ |E, l+1\rangle.$$

$A_l^+ |E, l+1\rangle$ is the eigenket of H_l with the eigenvalues $(E + \hbar\omega)$ and l .

$$A_l^+ |E, l+1\rangle \propto |E + \hbar\omega, l\rangle,$$

or

$$A_{l-1}^+ |E, l\rangle \propto |E + \hbar\omega, l-1\rangle.$$

$$A_{l-1}^+ |E, l\rangle \propto |E + \hbar\omega, l-1\rangle,$$

$$A_l |E, l\rangle \propto |E - \hbar\omega, l+1\rangle,$$

$$H_{l+1} |E - \hbar\omega, l+1\rangle = (E - \hbar\omega) |E - \hbar\omega, l+1\rangle,$$

$$H_l |E, l\rangle = E |E, l\rangle,$$

$$H_{l-1} |E + \hbar\omega, l-1\rangle = (E + \hbar\omega) |E + \hbar\omega, l-1\rangle.$$

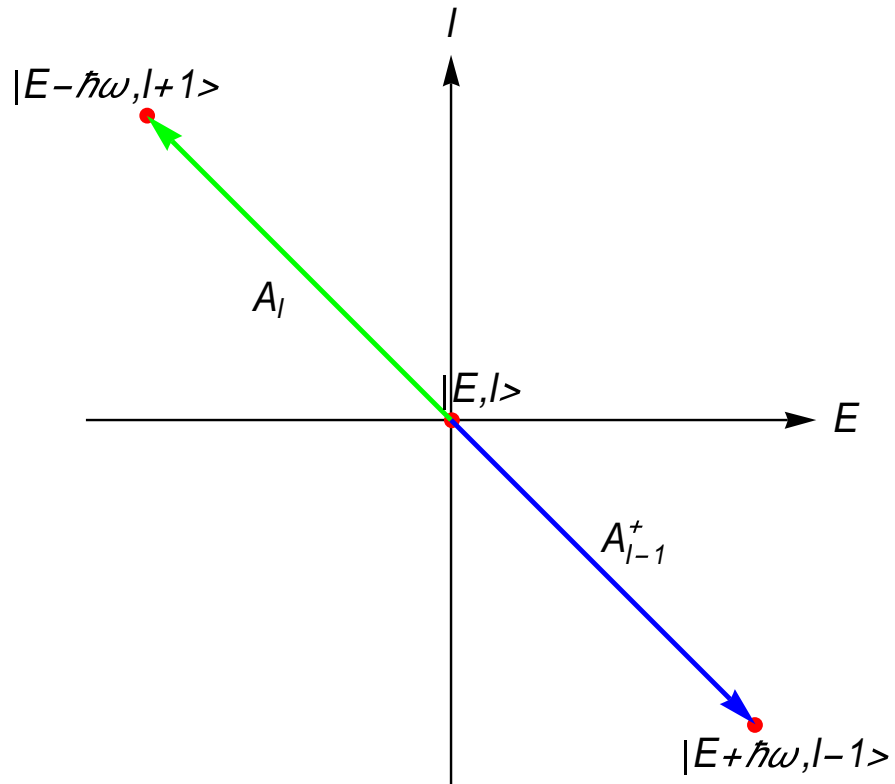


Figure helps to organize the generation of the radial wave functions. Each red circle represents the eigenstate. The degeneracy of the state with the quantum number l is $(2l+1)$.

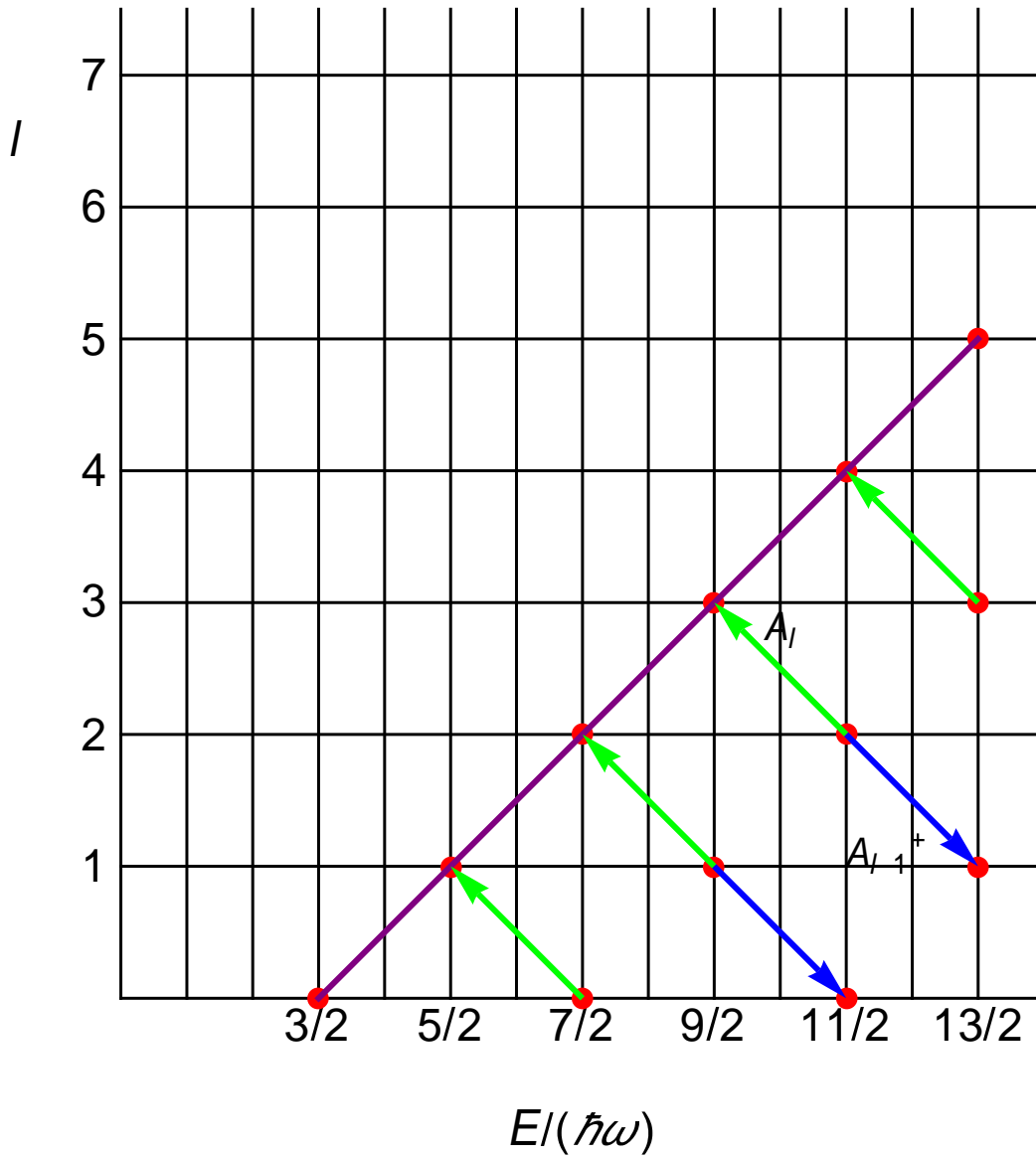


Fig. The allowed states denoted by red circles. in the $(E/(\hbar\omega), l)$ plane. The boundary line (purple line) is denoted by $E/(\hbar\omega) = (l + \frac{3}{2})$.

((Degeneracy))

$$E = \frac{3}{2}\hbar\omega \quad \text{degeneracy} = l \quad (l = 0)$$

$E = \frac{3}{2}\hbar\omega$	degeneracy = 1	($l = 0$)
		total states=1
$E = \frac{5}{2}\hbar\omega$	degeneracy = 3	($l = 1$)
		total states=3
$E = \frac{7}{2}\hbar\omega$	degeneracy = 1	($l = 0$)
	degeneracy = 5	($l = 2$)
		total states=6
$E = \frac{9}{2}\hbar\omega$	degeneracy = 3	($l = 1$)
	degeneracy = 7	($l = 3$)
		total states=10
$E = \frac{11}{2}\hbar\omega$	degeneracy = 1	($l = 0$)
	degeneracy = 5	($l = 2$)
	degeneracy = 9	($l = 4$)
		total states=15

APPENDIX
((Mathematica))

The quantum mechanical operator pr ;

The operator $A=AD$;

The operator $A+=AU$;

The Hamiltonian of 3D simple harmonics. μ is a reduced mass.

$$\begin{aligned} \text{Clear["Global`*"]}; \text{pr} &:= -i \frac{\hbar}{r} D[r \#, r] \& \\ \text{AD}[L_] &:= \frac{1}{\sqrt{2 \mu \hbar \omega}} \left(i \text{pr}[\#] - \frac{(L+1) \hbar}{r} \# + \mu \omega r \# \right) \& \\ \text{AU}[L_] &:= \frac{1}{\sqrt{2 \mu \hbar \omega}} \left(-i \text{pr}[\#] - \frac{(L+1) \hbar}{r} \# + \mu \omega r \# \right) \& \\ \text{H}[L_] &:= \left(\frac{1}{2 \mu} \text{pr}[\text{pr}[\#]] + \frac{L(L+1) \hbar^2}{2 \mu r^2} \# + \frac{\mu \omega^2}{2} r^2 \# \right) \& \end{aligned}$$

AI+ AI calculation

$$\begin{aligned} \text{f1} &= \text{AU}[L][\text{AD}[L][\chi[r]]] // \text{Simplify}; \\ \text{f2} &= \text{H}[L][\chi[r]] // \text{Simplify}; \\ \text{eq12} &= \left(\text{f1} - \frac{\text{f2}}{\hbar \omega} \right) // \text{Simplify} \\ &= -\frac{1}{2} (3 + 2L) \chi[r] \end{aligned}$$

The commutation relation

$$\text{AD}[L] \text{AU}[L] - \text{AU}[L] \text{AD}[L]$$

f3 = (AD[L][AU[L][χ[r]]] - AU[L][AD[L][χ[r]]]) // Simplify

$$\frac{(r^2 \mu \omega + \hbar + L \hbar) \chi[r]}{r^2 \mu \omega}$$

f4 = (H[L + 1][χ[r]] - H[L][χ[r]]) // Simplify)

$$\frac{(1 + L) \hbar^2 \chi[r]}{r^2 \mu}$$

eq34 = f3 - $\frac{f4}{\hbar \omega}$ // Simplify

$\chi[r]$

AD[L] H[L] - H[L]AD[L]

f5 = AD[L][H[L][χ[r]]] - H[L][AD[L][χ[r]]] // Simplify;

f6 = H[L + 1][AD[L][χ[r]]] - H[L][AD[L][χ[r]]] + $\hbar \omega$ AD[L][χ[r]] // Simplify;

eq56 = f5 - f6 // Simplify

0

AD[L] H[L] = H[L+1]AD[L]+ $\hbar\omega$ AD[L]

f7 = AD[L][H[L][χ[r]]] - H[L + 1][AD[L][χ[r]]] - $\hbar \omega$ AD[L][χ[r]] // Simplify

0