HW #9

1. 3D Harmonic Oscillator

(a) We handle the two terms separately; first the kinetic energy,

$$\left[L_i, \frac{\vec{p}^2}{2m}\right] = \epsilon_{ijk}[x_j\ p_k, \frac{p_l\ p_l}{2m}] = \epsilon_{ijk}[x_j, p_l\ p_l]\frac{p_k}{2m} = \epsilon_{ijk}\cdot 2\,i\hbar\,\delta_{jl}\ p_l\cdot\frac{p_k}{2m}$$
$$\Longrightarrow \propto \epsilon_{ijk}\ p_j\ p_k = 0$$

by antisymmetry of ϵ_{ijk}. Similarly the potential energy,

$$\left[L_i, \frac{1}{2}m\omega^2\vec{x}^2\right] = \epsilon_{ijk}\left[x_j\ p_k, \frac{1}{2}m\omega^2\ x_l\ x_l\right] = \epsilon_{ijk}\ x_j[p_k, x_l\ x_l]\frac{1}{2}m\omega^2$$
$$= \epsilon_{ijk}\ x_j\cdot 2\,(-i\hbar\,\delta_{kl}\ x_l)\cdot\frac{1}{2}m\omega^2 \Longrightarrow 0\,.$$

(b) We generalize the usual creation and annihilation operator for each spatial direction,

$$a_i = \sqrt{\frac{m\omega}{2\hbar}}\ (x_i + i\frac{p_i}{m\omega}), \qquad a_i{}^\dagger = \sqrt{\frac{m\omega}{2\hbar}}\ (x_i - i\frac{p_i}{m\omega})\,.$$

The commutation relations are obviously $[a_i, a_j{}^\dagger] = \delta_{ij}$. The Hamiltonian is simply the sum of three 1D harmonic oscillator Hamiltonians,

$$H = \hbar\,\omega\left(a_x{}^\dagger\ a_x + a_y{}^\dagger\ a_y + a_z{}^\dagger\ a_z + \frac{3}{2}\right).$$

The angular momentum operators are rewritten using

$$x_i = \sqrt{\frac{\hbar}{2m\omega}}\ (a_i + a_i{}^\dagger), \qquad p_i = -i\sqrt{\frac{\hbar m\omega}{2}}\ (a_i - a_i{}^\dagger)\,.$$

We find

$$L_i = \epsilon_{ijk}\ x_j\ p_k = \epsilon_{ijk}\sqrt{\frac{\hbar}{2m\omega}}\ (a_j + a_j{}^\dagger)\left(-i\sqrt{\frac{\hbar m\omega}{2}}\right)(a_k - a_k{}^\dagger)$$
$$= -i\frac{\hbar}{2}\epsilon_{ijk}(a_j + a_j{}^\dagger)(a_k - a_k{}^\dagger)$$
$$= -i\frac{\hbar}{2}\epsilon_{ijk}(a_j\ a_k - a_j\ a_k{}^\dagger + a_j{}^\dagger\ a_k - a_j{}^\dagger\ a_k{}^\dagger)$$
$$= -i\frac{\hbar}{2}\epsilon_{ijk}(a_j{}^\dagger\ a_k - a_k{}^\dagger\ a_j)$$
$$L_i = -i\hbar\,\epsilon_{ijk}\ a_j{}^\dagger\ a_k\,.$$

For later purposes, it is useful to define

$$a_+ = \frac{-1}{\sqrt{2}}(a_x - i\,a_y), \quad a_- = \frac{1}{\sqrt{2}}(a_x + i\,a_y)\,.$$

Note that

$$[a_+, a_+{}^\dagger] = [a_-, a_-{}^\dagger] = 1,$$
$$[a_+, a_-] = [a_+, a_-{}^\dagger] = [a_+{}^\dagger, a_-] = [a_+{}^\dagger, a_-{}^\dagger] = 0\,.$$

Then the angular momentum operators can be further rewritten as

$$L_+ = L_x + i L_y = -i\hbar(a_y^\dagger a_z - a_z^\dagger a_y) + \hbar(a_z^\dagger a_x - a_x^\dagger a_z)$$
$$= \hbar(-(a_x^\dagger + i a_y^\dagger) a_z + a_z^\dagger (a_x + i a_y))$$
$$L_+ = \hbar\sqrt{2}\,(a_+^\dagger a_z + a_z^\dagger a_-)$$

$$L_- = L_x - i L_y = -i\hbar(a_y^\dagger a_z - a_z^\dagger a_y) - \hbar(a_z^\dagger a_x - a_x^\dagger a_z)$$
$$= \hbar((a_x^\dagger - i a_y^\dagger) a_z - a_z^\dagger (a_x - i a_y))$$
$$L_- = \hbar\sqrt{2}\,(a_-^\dagger a_z + a_z^\dagger a_+)$$

$$L_z = -i\hbar\,(a_x^\dagger a_y - a_y^\dagger a_x) = -i\hbar\left(\frac{a_-^\dagger - a_+^\dagger}{\sqrt{2}}\,\frac{a_- + a_+}{\sqrt{2}\,i} - \frac{a_-^\dagger + a_+^\dagger}{-\sqrt{2}\,i}\,\frac{a_- - a_+}{\sqrt{2}}\right)$$
$$L_z = \hbar(a_+^\dagger a_+ - a_-^\dagger a_-)\,.$$

In other words, $a_+^\dagger$ (a_+) creates (annihilates) the excitation with $L_z = +\hbar$, while $a_-^\dagger$ (a_-) creates (annihilates) one with $L_z = -\hbar$.

(c) The ground state is unique, and the only representation of angular momentum that can be formed by a single state is $l = 0$.

A more explicit way to show it is simply by acting

$$L_+ \,|0\rangle = \hbar\sqrt{2}\,(a_+^\dagger a_z + a_z^\dagger a_-)\,\big|0\big\rangle = 0,$$

$$L_- \,|0\rangle = \hbar\sqrt{2}\,(a_-^\dagger a_z + a_z^\dagger a_+)\,\big|0\big\rangle = 0,$$

$$L_z \,|0\rangle = \hbar(a_+^\dagger a_+ - a_-^\dagger a_-)\,|0\rangle = 0.$$

(d) The creation operators are $k = 1$ spherical tensor operators,

$$T_{+1}^{(1)} = a_+^\dagger,\ T_0^{(1)} = a_z^\dagger,\quad T_{-1}^{(1)} = a_-^\dagger.$$

To verify this claim:

$$\left[L_+,\, T_{+1}^{(1)}\right] = \left[\hbar\sqrt{2}\,(a_+^\dagger a_z + a_z^\dagger a_-),\, a_+^\dagger\right] = 0,$$

$$\left[L_-,\, T_{+1}^{(1)}\right] = \left[\hbar\sqrt{2}\,(a_-^\dagger a_z + a_z^\dagger a_+),\, a_+^\dagger\right] = \hbar\sqrt{2}\,a_z^\dagger = \hbar\sqrt{2}\,T_0^{(1)},$$

$$\left[L_-,\, T_0^{(1)}\right] = \left[\hbar\sqrt{2}\,(a_-^\dagger a_z + a_z^\dagger a_+),\, a_z^\dagger\right] = \hbar\sqrt{2}\,a_-^\dagger = \hbar\sqrt{2}\,T_{-1}^{(1)},$$

$$\left[L_-,\, T_{-1}^{(1)}\right] = \left[\hbar\sqrt{2}\,(a_-^\dagger a_z + a_z^\dagger a_+),\, a_+^\dagger\right] = 0\,.$$

Indeed, the operators form the $k = 1$ representation.

(e) Using the notation defined above,

$$|1,\,1,\,\pm 1\rangle = a_\pm^\dagger\,|0\rangle.$$

First we show that $|1,\,1,\,1\rangle$ cannot be raised:

$$L_+ \,|1,\,1,\,1\rangle = \hbar\sqrt{2}\,(a_+^\dagger a_z + a_z^\dagger a_-)\,a_+^\dagger\,\big|0\big\rangle = 0.$$

Then by lowering this state,

$$L_- \,|\,1,\,1,\,1\rangle = \hbar\sqrt{2}\,(a_-{}^\dagger\,a_z + a_z{}^\dagger\,a_+)\,a_+{}^\dagger\,\big|0\big\rangle = \hbar\sqrt{2}\,a_z{}^\dagger\,\big|0\big\rangle = \hbar\sqrt{2}\,\big|1,\,1,\,0\big\rangle.$$

Lowering this state once more,

$$L_- \,|\,1,\,1,\,0\rangle = \hbar\sqrt{2}\,(a_-{}^\dagger\,a_z + a_z{}^\dagger\,a_+)\,a_z{}^\dagger\,\big|0\big\rangle = \hbar\sqrt{2}\,a_-{}^\dagger\,\big|0\big\rangle = \hbar\sqrt{2}\,\big|1,\,1,\,-1\big\rangle.$$

Finally this state cannot be lowered

$$L_- \,|\,1,\,1,\,-1\rangle = \hbar\sqrt{2}\,(a_-{}^\dagger\,a_z + a_z{}^\dagger\,a_+)\,a_-{}^\dagger\,\big|0\big\rangle = 0.$$

Therefore, they form the $l = 1$ representation correctly.

(f) We first rewrite the quadrupole moment operator in terms of creation and annihilation operators. Starting with $x_i = \sqrt{\frac{\hbar}{2\,m\,\omega}}\,(a_i + a_i{}^\dagger)$,

$$\begin{aligned}
3\,z^2 - r^2 &= 2\,z^2 - x^2 - y^2 = \frac{\hbar}{2\,m\,\omega}\left(2\,(a_z + a_z{}^\dagger)^2 - (a_x + a_x{}^\dagger)^2 - (a_y + a_y{}^\dagger)^2\right)\\
&= \frac{\hbar}{2\,m\,\omega}\left(2\,(a_z + a_z{}^\dagger)^2 - \left(\frac{a_- - a_+}{\sqrt{2}} + \frac{a_-{}^\dagger - a_+{}^\dagger}{\sqrt{2}}\right)^2 - \left(\frac{a_- + a_+}{\sqrt{2}\,i} + \frac{a_-{}^\dagger + a_+{}^\dagger}{-\sqrt{2}\,i}\right)^2\right).
\end{aligned}$$

Because we will take the expectation values of this operator, we are only interested in the pieces with one creation and one annihilation operators. The pieces with two creation or two annihilation operators do not give non−vanishing expectation values. Therefore keeping only those terms,

$$\begin{aligned}
3\,z^2 - r^2 \sim{}& \frac{\hbar}{2\,m\,\omega}\Big(2\,(a_z\,a_z{}^\dagger + a_z{}^\dagger\,a_z)\\
&- \frac{1}{2}\,((a_- - a_+)\,(a_-{}^\dagger - a_+{}^\dagger) + (a_-{}^\dagger - a_+{}^\dagger)\,(a_- - a_+))\\
&- \frac{1}{2}\,((a_- + a_+)\,(a_-{}^\dagger + a_+{}^\dagger) + (a_-{}^\dagger + a_+{}^\dagger)\,(a_- + a_+))\Big)\\
={}& \frac{\hbar}{2\,m\,\omega}\,(2\,(a_z\,a_z{}^\dagger + a_z{}^\dagger\,a_z) - (a_-\,a_-{}^\dagger + a_-{}^\dagger\,a_- + a_+\,a_+{}^\dagger + a_+{}^\dagger\,a_+))\\
={}& \frac{\hbar}{m\,\omega}\,(2\,a_z{}^\dagger\,a_z - (a_-{}^\dagger\,a_- + a_+{}^\dagger\,a_+)).
\end{aligned}$$

In the last step, we used the commutation relation to rewrite $a\,a^\dagger = a^\dagger\,a + 1$, and cancelled the constant pieces against each other. Then it is easy to work out the expectation values,

$$\langle 1,\,1,\,1\,|\,3\,z^2 - r^2\,|\,1,\,1,\,1\rangle = \left\langle 0\,\middle|\,a_+\,\frac{\hbar}{m\,\omega}\,(2\,a_z{}^\dagger\,a_z - (a_-{}^\dagger\,a_- + a_+{}^\dagger\,a_+))\,a_+{}^\dagger\,\middle|\,0\right\rangle = -\frac{\hbar}{m\,\omega},$$

$$\langle 1,\,1,\,0\,|\,3\,z^2 - r^2\,|\,1,\,1,\,0\rangle = \left\langle 0\,\middle|\,a_z\,\frac{\hbar}{m\,\omega}\,(2\,a_z{}^\dagger\,a_z - (a_-{}^\dagger\,a_- + a_+{}^\dagger\,a_+))\,a_z{}^\dagger\,\middle|\,0\right\rangle = 2\,\frac{\hbar}{m\,\omega},$$

$$\langle 1,\,1,\,-1\,|\,3\,z^2 - r^2\,|\,1,\,1,\,-1\rangle = \left\langle 0\,\middle|\,a_-\,\frac{\hbar}{m\,\omega}\,(2\,a_z{}^\dagger\,a_z - (a_-{}^\dagger\,a_- + a_+{}^\dagger\,a_+))\,a_-{}^\dagger\,\middle|\,0\right\rangle = -\frac{\hbar}{m\,\omega}.$$

The quadrupole moment operator here is a spherical tensor operator with $k = 2$, $q = 0$. To see if this result is consistent with the Wigner−Eckart theorem, we need the Clebsch−Gordan coefficients

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Table[ClebschGordan[{1, m}, {2, 0}, {1, m}], {m, -1, 1}]
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$$\left\{\frac{1}{\sqrt{10}},\ -\sqrt{\frac{2}{5}},\ \frac{1}{\sqrt{10}}\right\}$$

The ratios among the expectation values are indeed the same as the ratios among the Clebsch−Gordan coefficients, $1:-2:1$.

As an added note, a positive quadrupole moment $\langle 3z^2 - r^2 \rangle > 0$ indicates a prolate form, while a negative quadrupole moment $\langle 3z^2 - r^2 \rangle < 0$ indicates an oblated form.

(g) From part (d), we can surmise that the six states are composed of: $(a_+^\dagger)^2 \left|0\right\rangle$, $(a_z^\dagger)^2 \left|0\right\rangle$, $(a_-^\dagger)^2 \left|0\right\rangle$, $a_+^\dagger a_z^\dagger \left|0\right\rangle$, $a_+^\dagger a_-^\dagger \left|0\right\rangle$, $a_z^\dagger a_-^\dagger \left|0\right\rangle$. By looking at the L_z eigenvalues, it is easy to identify

$$\left|2, 2, 2\right\rangle = \frac{1}{\sqrt{2}} (a_+^\dagger)^2 \left|0\right\rangle,$$

$$\left|2, 2, 1\right\rangle = a_+^\dagger a_z^\dagger \left|0\right\rangle,$$

$$\left|2, 2, -1\right\rangle = a_z^\dagger a_-^\dagger \left|0\right\rangle,$$

$$\left|2, 2, -2\right\rangle = \frac{1}{\sqrt{2}} (a_-^\dagger)^2 \left|0\right\rangle .$$

There are two states with $m = 0$: $(a_z^\dagger)^2 \left|0\right\rangle$, $a_+^\dagger a_-^\dagger \left|0\right\rangle$. We can tell which linear combination belongs to $l = 2$ representation by acting L_- on $\left|2, 2, 1\right\rangle$,

$$\begin{aligned} L_- \left|2, 2, 1\right\rangle &= \hbar \sqrt{2} \, (a_-^\dagger a_z + a_z^\dagger a_+) \, a_+^\dagger a_z^\dagger \left|0\right\rangle = \hbar \sqrt{2} \, (a_-^\dagger a_+^\dagger + a_z^\dagger a_z^\dagger) \left|0\right\rangle \\ &= \hbar \sqrt{6} \left|2, 2, 0\right\rangle . \end{aligned}$$

Therefore, we can identify

$$\left|2, 2, 0\right\rangle = \frac{1}{\sqrt{3}} (a_-^\dagger a_+^\dagger + a_z^\dagger a_z^\dagger) \left|0\right\rangle$$

which is properly normalized as it should be. The orthogonal combination is

$$\left|2, 0, 0\right\rangle = \frac{1}{\sqrt{6}} (2 a_-^\dagger a_+^\dagger - a_z^\dagger a_z^\dagger) \left|0\right\rangle .$$

To verify that this state is indeed an $l = 0$ state, we can check

$$\begin{aligned} L_+ \left|2, 0, 0\right\rangle &= \hbar \sqrt{2} \, (a_+^\dagger a_z + a_z^\dagger a_-) \, \frac{1}{\sqrt{6}} (2 a_-^\dagger a_+^\dagger - a_z^\dagger a_z^\dagger) \left|0\right\rangle \\ &= \hbar \sqrt{2} \, \frac{1}{\sqrt{6}} (-a_+^\dagger a_z^\dagger - a_z^\dagger a_+^\dagger + 2 a_z^\dagger a_+^\dagger) \left|0\right\rangle = 0 . \end{aligned}$$

A much more systematic way of obtaining the same result is to use Sakurai's Eq. (3.10.27). Even though this example is simple enough to work it out explicitly as done above, the generalization to higher N would be quite cumbersome.

Eq. (3.10.27) says

$$\begin{aligned} T_0^{(2)} &= \sum\nolimits_{q_1, q_2} \langle 1\,1; q_1, q_2 \,|\, 2\,0\rangle \, T_{q_1}^{(1)} \, T_{q_2}^{(1)} \\ &= \langle 1\,1; +1\ -1 \,|\, 2\,0\rangle \, T_{+1}^{(1)} \, T_{-1}^{(1)} + \langle 1\,1; 0\,0 \,|\, 2\,0\rangle \, T_0^{(1)} \, T_0^{(1)} + \langle 1\,1; -1\ +1 \,|\, 2\,0\rangle \, T_{-1}^{(1)} \, T_{+1}^{(1)} \\ &= \frac{1}{\sqrt{6}} a_+^\dagger a_-^\dagger + \sqrt{\frac{2}{3}} \, a_z^\dagger a_z^\dagger + \frac{1}{\sqrt{6}} a_-^\dagger a_+^\dagger \\ &= \sqrt{\frac{2}{3}} \, (a_-^\dagger a_+^\dagger + a_z^\dagger a_z^\dagger) . \end{aligned}$$

Therefore, the operator $(a_-^\dagger a_+^\dagger + a_z^\dagger a_z^\dagger)$ creates an $l = 2$ state. Similarly,

$$T_0^{(0)} = \sum_{q_1,q_2} \langle 1\,1;\, q_1,\, q_2 \,|\, 0\,0\rangle\, T_{q_1}^{(1)}\, T_{q_2}^{(1)}$$
$$= \langle 1\,1;\, +1\, -1 \,|\, 0\,0\rangle\, T_{+1}^{(1)}\, T_{-1}^{(1)} + \langle 1\,1;\, 0\,0 \,|\, 0\,0\rangle\, T_0^{(1)}\, T_0^{(1)} + \langle 1\,1;\, -1\, +1 \,|\, 0\,0\rangle\, T_{-1}^{(1)}\, T_{+1}^{(1)}$$
$$= \frac{1}{\sqrt{3}}\, a_+^\dagger\, a_-^\dagger - \frac{1}{\sqrt{3}}\, a_z^\dagger\, a_z^\dagger + \frac{1}{\sqrt{3}}\, a_-^\dagger\, a_+^\dagger$$
$$= \frac{1}{\sqrt{3}}\,(2\, a_-^\dagger\, a_+^\dagger - a_z^\dagger\, a_z^\dagger) = -\frac{1}{\sqrt{3}}\,(a_x^\dagger\, a_x^\dagger + a_y^\dagger\, a_y^\dagger + a_z^\dagger\, a_z^\dagger) = -\frac{1}{\sqrt{3}}\,\vec{a}^\dagger\cdot\vec{a}^\dagger\,.$$

The last expression shows it is manifestly rotation invariant. Therefore, the operator $(2\, a_-^\dagger\, a_+^\dagger - a_z^\dagger\, a_z^\dagger)$ creates an $l = 0$ state. The rest of the job is to properly normalize the states, reproducing the above results.

(h) For $N = 3$, it is clear that the state with the highest L_z eigenvalue is $(a_+^\dagger)^3\,|0\rangle$ with $m = 3$. Hence, it belongs to the $l = 3$ representation, which has $2\,l + 1 = 7$ states. The only one way to create an $m = 2$ state is $a_z\,(a_+^\dagger)^2\,|0\rangle$, so there is no orthogonal $l = 2$ representation. However, there are two $m = 1$ states $(a_+^\dagger)^2\, a_-^\dagger\,|0\rangle$ and $(a_z^\dagger)^2\, a_-^\dagger\,|0\rangle$, so there is an orthogonal $l = 1$ representation with 3 states. Finally, there are only two ways to make an $m = 0$ state, $(a_z^\dagger)^3\,|0\rangle$ and $a_z^\dagger\, a_+^\dagger\, a_-^\dagger\,|0\rangle$, so there is not an additional $l = 0$ representation. Thus, there are 10 states in total.

Similarly, for $N = 4$, the highest representation must be $l = 4$ with 9 states. Learning from above, there are only three ways to make $m = 0$: $(a_+^\dagger)^2\,(a_-^\dagger)^2\,|0\rangle$, $(a_z^\dagger)^2\, a_+^\dagger\, a_-^\dagger\,|0\rangle$, and $(a_z^\dagger)^4\,|0\rangle$, so there are three total representations. The only $m = 3$ state is $a_z^\dagger\,(a_+^\dagger)^3\,|0\rangle$, so there is no $l = 3$; there are two $m = 2$ states $(a_+^\dagger)^3\, a_-^\dagger\,|0\rangle$ and $a_z^\dagger\,(a_+^\dagger)^2\,|0\rangle$, so there is an $l = 2$ representation with 5 states. The final representation must be $l = 0$ with one state. This gives 15 states in total.

(i) [optional] We note that the creation operators are linear combinations of $\vec{x}$ and $\vec{p}$ and hence parity odd. Therefore, $N =$ even states have even parity, and hence can only have even l, while $N =$ odd states odd parity, and hence odd l. In general, $N =$ even states have $l = 0,\ 2,\ \cdots,\ N$, while $N =$ odd states have $l = 1,\ 3,\ \cdots,\ N$. It can be verified by looking at the number of states. (We will prove parity below.)

The number of states at level N is the number of ways to make N selections of the three objects $a_z^\dagger$, $a_+^\dagger$ and $a_-^\dagger$ with replacement. We may use the "multiset" ${}_3H_N = {}_{N+2}C_N = (N+2)\,(N+1)/2$. For even $N = 2\,k$, it is $(k+1)\,(2\,k+1)$. Each $l = 2\,j$ contributes $2\,l + 1 = 4\,j + 1$ states, and the total is $\sum_{j=0}^{k}(4\,j+1) = 2\,k(k+1) + (k+1) = (k+1)\,(2\,k+1)$. For odd $N = 2\,k-1$, the number of states is $k(2\,k+1)$. Each $l = 2\,j-1$ contributes $2\,l + 1 = 4\,j - 1$ states, and the total is $\sum_{j=1}^{k}(4\,j-1) = 2\,k(k+1) - k = k(2\,k+1)$.

(j) [optional] Recognizing that $\vec{a}^\dagger\cdot\vec{a} = N$ is Hermitian, i.e. $\left(\vec{a}^\dagger\cdot\vec{a}\right)^\dagger = \left(\vec{a}\right)^\dagger\cdot\left(\vec{a}^\dagger\right)^\dagger = \vec{a}^\dagger\cdot\vec{a}$, we may use the Baker−Hausdorff formula to evaluate the expression:

$$\Pi\,\vec{x}\,\Pi^\dagger = e^{i\pi N}\cdot\sqrt{\frac{\hbar}{2\,m\,\omega}}\left(\vec{a}+\vec{a}^\dagger\right)\cdot e^{-i\pi N} = \sqrt{\frac{\hbar}{2\,m\,\omega}}\sum_m \frac{(i\,\pi)^m}{m!}\Big[N,\Big[N,\Big[N,\ \ldots\Big[N,\,\vec{a}+\vec{a}^\dagger\Big]\ldots\Big]\Big]\Big]_m\,.$$

Noting that $[N,\, a^{(\dagger)}] = \mp a^{(\dagger)}$ we may collapse this result and separate the even and odd terms:

$$\Pi\,\vec{x}\,\Pi^\dagger = \sqrt{\frac{\hbar}{2\,m\,\omega}}\sum_m \frac{(i\,\pi)^m}{m!}\left((-1)^m\,\vec{a}+\vec{a}^\dagger\right) = \sqrt{\frac{\hbar}{2\,m\,\omega}}\left(\left(\vec{a}+\vec{a}^\dagger\right)\cos(\pi) + \left(-\vec{a}+\vec{a}^\dagger\right)\sin(\pi)\right)$$

$$\Longrightarrow \Pi\,\vec{x}\,\Pi^\dagger = -\vec{x}\,.$$

$\Pi\,\vec{p}\,\Pi^\dagger = -\vec{p}$ follows immediately with $\vec{x} \to \vec{p} = -i\sqrt{\frac{\hbar\,m\,\omega}{2}}\left(\vec{a}-\vec{a}^\dagger\right)$ since only the odd term changes a sign.

(k) The computation is trivial:

$$\Pi \,|\, N,\, l,\, m\rangle \;=\; e^{i\,\pi\,\vec{a}^{\dagger}\,\vec{a}} \;\Big|\; N,\, l,\, m\Big\rangle \Longrightarrow \Pi = e^{i\,\pi\,N} \;=\; (e^{i\,\pi})^{N} \;=\; (-1)^{N}\;.$$

(l) Considering only the Wigner−Eckhart theorem, a $2\,P \to 1\,P$ transition is allowed since $\Delta\, l = 0$ and $l \neq 0$. However, we note that $2\,P$ and $1\,P$ are both parity−odd eigenstates (which belong to odd N levels, as we have proved). The dipole operator is parity−odd, so the amplitude of the transition is zero by parity conservation. A parity−odd operator can only connect states of opposite parity under conservation.

2. Rectangular Double−Well Potential

Overview:

Because the potential is infinite for $|\,x\,| \,>\, a + b$, the wave function should vanish at $x = \pm\,(a + b)$.

For $a < x < a + b$ and $-a - b < x < -a$, the potential vanishes and the wave function is given simply by a plane wave $e^{\pm\,i\,k\,x}$ with energy $E = \hbar^2\; k^2\;/\,2\,m$.

For $-a < x < a$, the potential is large V_0, and the wave function damps exponentially, $e^{\pm\kappa\,x}$ with $\hbar^2\;\kappa^2 \;= 2\,m(V_0 \,-\, E) = 2\,m\,V_0 \,-\, \hbar^2\;k^2$.

Because the potential is parity−invariant $V(-x) = V(x)$, we expect the ground state to be a symmetric (parity−even) function, with a close excited state with an anti−symmetric (parity−odd) wave function.

Parity−even ground state:

The wave function for $-a < x < a$ must be $\psi(x) = A\cosh\kappa\,x$.

For $a < |\,x\,| \,< a + b$, the wave function must be $\psi(x) = B\sin k(x - a - b)$ to ensure the boundary condition at $|\,x\,| = a + b$. For $-a - b < x < -a$, $\psi(x) = \psi(-x) = -B\sin k(x + a + b)$.

To match the logarithmic derivative $\psi\,'\,(a)\,/\,\psi(a)$, we need $\frac{\psi\,'\,(a)}{\psi(a)} = \kappa\tanh\kappa\,a = k\cot k(-b)$. The condition at $x = -a$ is precisely the same due to the parity.

Parity−odd excited state:

The wave function for $-a < x < a$ must be $\psi(x) = A\sinh\kappa\,x$.

For $a < x < a + b$, the wave function must be $\psi(x) = B\sin k(x - a - b)$ to ensure the boundary condition at $|\,x\,| = a + b$.

For $-a - b < x < -a$, $\psi(x) = -\psi(-x) = B\sin k(x + a + b)$.

To match the logarithmic derivative $\psi\,'\,(a)\,/\,\psi(a)$, we need $\frac{\psi\,'\,(a)}{\psi(a)} = \kappa\coth\kappa\,a = k\cot k(-b)$. The condition at $x = -a$ is precisely the same thanks to the parity.

Energy splitting:

First we take the limit of the inifinite potenital barrier $V_0 \to \infty$, and hence $\kappa \to \infty$. Then $\coth\kappa\,a = \tanh\kappa\,a = 1$, and the condition is $-k\,a\cot k\,b = \kappa\,a \to \infty$. The only way to satisfy this equation is by taking $k\,b \;=\; (2\,n + 1)\,\pi$ so that $\cot k\,b \to -\infty$. The lowest energy is obtained by $k\,b = \pi$. Namely, to the leading order in large V_0, $k = \frac{\pi}{b}$ and $E = \frac{\hbar^2\,\pi^2}{2\,m\,b^2}$ for both parity−even and odd states. This makes sense because the wave function fits right in between two infinite potential

barriers.

Now we make the potential barrier finite but large ($\kappa a \gg 1$), and the two states split. To see the difference between two energy levels, we note that the only difference is between $\tanh \kappa a$ and $\coth \kappa a$, and for a large $\kappa a \gg 1$, the difference is exponentially small,

$$\tanh \kappa a = 1 - 2\, e^{-2\kappa a} + O(e^{-4\kappa a}), \qquad \coth \kappa a = 1 + 2\, e^{-2\kappa a} + O(e^{-4\kappa a})\ .$$

Therefore we would like to solve $\kappa a\,(1 \mp 2\, e^{-2\kappa a}) = -k a \cot k b$ to find $k \simeq \frac{\pi}{b}$ for parities ± 1. We expand $k b = \pi - \epsilon$, and

$$-k a \cot k b = \frac{-k a \cos k b}{\sin k b} = \frac{k a}{\epsilon} + O(\epsilon) = \frac{\pi a}{b \epsilon} + O(\epsilon^0),$$

and hence

$$\frac{\pi a}{b \epsilon} = \kappa a (1 \mp 2\, e^{-2\kappa a}), \qquad \epsilon = \frac{\pi}{\kappa b}\,(1 \pm 2\, e^{-2\kappa a})\ .$$

Therefore the energy eigenvalue is

$$E = \frac{\hbar^2 \pi^2}{2 m b^2}\left(1 - 2\,\frac{1}{\kappa b}\,(1 \pm 2\, e^{-2\kappa a})\right)$$

to leading order. The difference in the energies between the two low−lying states is exponentially suppressed as expected,

$$\Delta E = \frac{\hbar^2 \pi^2}{2 m b^2}\,\frac{8}{\kappa b}\, e^{-2\kappa a}.$$

Note that the exponential suppression in the energy difference $e^{-2\kappa a}$ is precisely the WKB factor in the limit $V_0 \gg E$, $\exp\left(-\frac{1}{\hbar}\int_{-a}^{a}\sqrt{2\,m(V-E)}\;dx\right) = \exp\left(-\frac{1}{\hbar}\,\sqrt{2\,m\,V_0}\;2\,a\right) = e^{-2\kappa a}$, verifying the origin of the energy splitting due to the tunneling between two minima.

Plot the wave functions:

We choose $a = b = 1$, $m = 1$, $\hbar = 1$, and $V_0 = 10$. Much larger V_0 makes it impossible to find the difference between the two energy eigenvalues numerically. We can solve numerically for k,

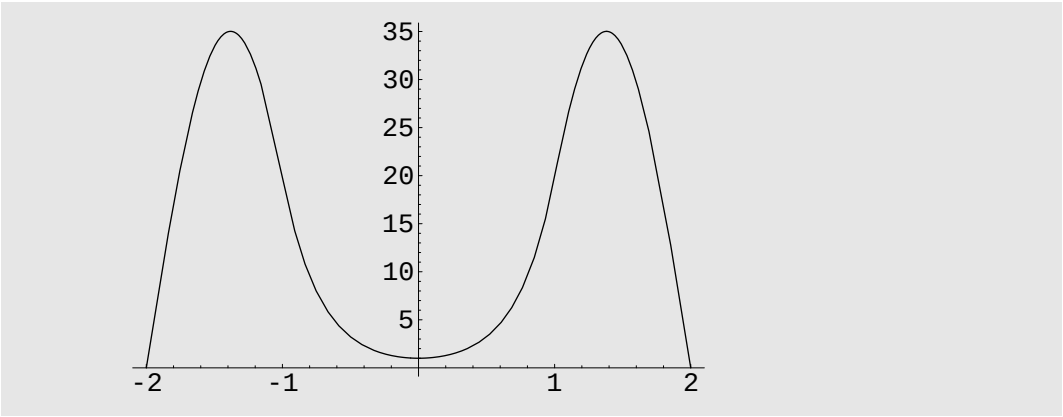
```
keqe = κ Tanh[κ a] == -k Cot[k b] /. {κ -> Sqrt[2 m V₀ - k²]} /. {ħ → 1, a → 1, b → 1, m → 1, V₀ → 10};

kroote = FindRoot[keqe, {k, 3}];

ksole = k /. kroote
```

```
2.53762
```

```
Plot[If[Abs[x] < 1, Cosh[Sqrt[20 - ksole^2] x],
    Cosh[Sqrt[20 - ksole^2]] / Sin[ksole (Abs[1] - 2)] Sin[ksole (Abs[x] - 2)]], {x, -2, 2}];
```



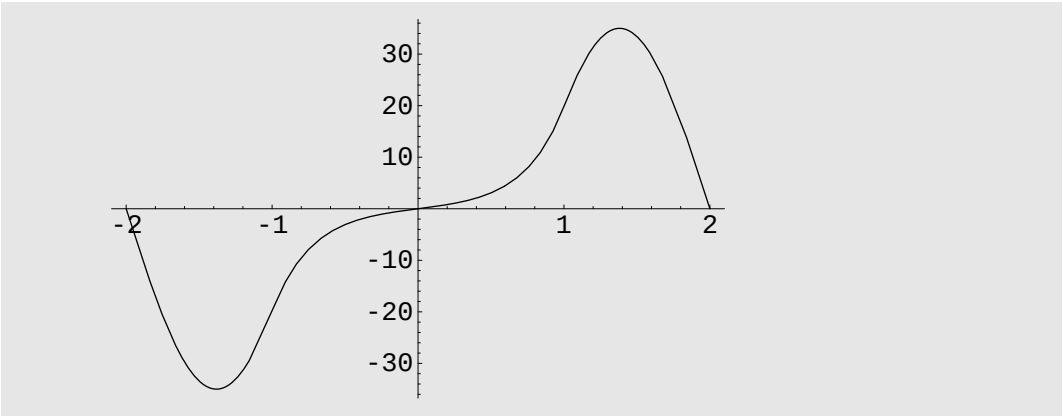

```
keqo = κ Coth[κ a] == -k Cot[k b] /. {κ -> Sqrt[2 m V0 - k^2]} /. {ħ → 1, a → 1, b → 1, m → 1, V0 → 10};

krooto = FindRoot[keqo, {k, 3}];

ksolo = k /. krooto
```

```
2.53855
```

```
Plot[If[Abs[x] < 1, Sinh[Sqrt[20 - ksolo^2] x],
    Sign[x] Sinh[Sqrt[20 - ksolo^2]] / Sin[ksolo (Abs[1] - 2)] Sin[ksolo (Abs[x] - 2)]], {x, -2, 2}];
```



3. [optional] Rotation Spectra of Diatomic Molecules

The vibrational splittings are smaller than the rotational splittings, so we pick out the transition frequencies at the vibrational ground state "0" as suggested; for $^{12}C\,^{32}S$ in MHz:

```
freqs1232 = {48990.973, 97980.950, 146969.033, 195954.226, 244935.737,
   293912.244, 342883.000, 391847.030, 440803.392, 489751.040, 538688.830};
```

We ignore the uncertainties since they are so small compared to the differences between adjacent frequencies.

The energy splitting is

$$E_j - E_{j-1} = \frac{J^2}{2I} = \frac{\hbar^2}{2I}\,(j(j+1) - (j-1)\,(j-1+1)) = \frac{\hbar^2}{2I}\,(j^2 + j - j^2 + j)$$
$$= \frac{\hbar^2}{I}\,j = \hbar(2\,\pi\,f)$$

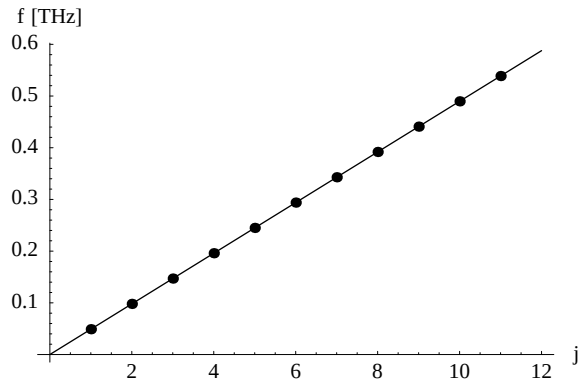
so we expect the frequency of the downward splitting of state j to be $f_j = \frac{\hbar}{2\pi I}\,j$ for some moment I. Let us implement fitting and plotting routines:

```
fitfunc[j_] = ħ/(2 π I0) j /. ħ → 1.05457148 * 10^-34;
Ifit[freqs_] := I0 /. FindFit[freqs * 10^6, fitfunc[j], {{I0, 10^-34 / 10^11}}, {j}];
plotfit[freqs_, If_] := Show[
   Plot[
    fitfunc[j] / 10^12 /. I0 → If, {j, 0, Length[freqs] + 1},
    AxesOrigin → {0, 0}, AxesLabel → TraditionalForm /@ {"j", "f [THz]"},
    TextStyle → {FontFamily -> "Times", FontSize → 8},
    DisplayFunction → Identity
   ],
   ListPlot[
    freqs / 10^6, Axes → False,
    PlotStyle → PointSize[0.02],
    DisplayFunction → Identity
   ],
   DisplayFunction → $DisplayFunction
  ];
```

Let us now perform the fit and plot the result:

```
I1232 = Ifit[freqs1232]
plotfit[freqs1232, I1232];
```

```
3.42682 × 10^-46
```



We obtain perfect linearity, showing the accuracy of the model given. This fit results in a moment of inertia $I = 3.43 \times 10^{-46}\ \mathrm{kg \cdot m^2}$. What is the interatomic distance that corresponds to this moment? We can try a classical "barbell" model for the molecule about the center of mass:

$$I = m_1\,{r_1}^2 + m_2\,{r_2}^2\,,\quad m_1\,r_1 = m_2\,r_2\,,\qquad R = r_1 + r_2$$

$$\Longrightarrow r_1 = \frac{m_2}{m_1} r_2 \Longrightarrow I = m_1 \left(\frac{m_2}{m_1} r_2\right)^2 + m_2 {r_2}^2 \Longrightarrow r_2 = \sqrt{I\left(\frac{{m_2}^2}{m_1} + m_2\right)^{-1}}$$

$$\Longrightarrow R = \left(\frac{m_2}{m_1} + 1\right)\sqrt{I \frac{m_1}{{m_2}^2 + m_1 m_2}} = \sqrt{I \frac{m_1}{m_2 (m_1 + m_2)} \left(\frac{m_1 + m_2}{m_1}\right)^2}$$

$$R = \sqrt{I \frac{m_1 + m_2}{m_1 m_2}} \ .$$

(We find $I = \mu R^2$ where μ is the reduced mass, as one would expect from co−orbiting bodies.) Let us compute:

```
Rmol[I0_, m1_, m2_] = Sqrt[I0 (m1 + m2)/(m1 * m2) / (1.66 * 10^-27)];
R1232 = Rmol[I1232, 12, 32]
```

```
1.53799 × 10^-10
```

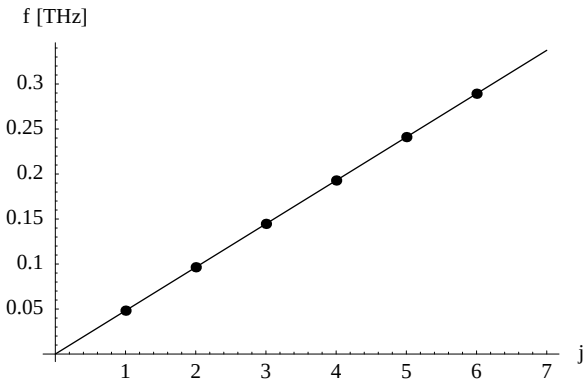
We find that $R \simeq 1.54$ Å for ${}^{12}C\,{}^{32}S$. According to Wikipedia, the covalent bond radii of carbon and sulfur are 0.77 Å and 1.02 Å respectively, so this result is in the ballpark. Furthermore, the barbell model should be decent because the vibrational mode is fairly stiff and the mass is well−localized in the nuclei.

Let us proceed to run the numbers for ${}^{12}C\,{}^{34}S$:

```
freqs1234 = {48206.915, 96412.940, 144617.109, 192818.464, 241016.194, 289209.230};
I1234 = Ifit[freqs1234]
R1234 = Rmol[I1234, 12, 34]
plotfit[freqs1234, I1234];
```

```
3.48193 × 10^-46
```

```
1.53782 × 10^-10
```

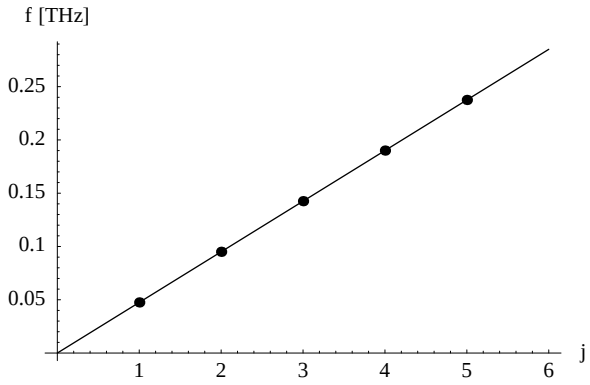


And for ${}^{12}C\,{}^{36}S$:

```
freqs1236 = {47508.819, 95016.722, 142522.785, 190026.190, 237526.008};
I1236 = Ifit[freqs1236]
R1236 = Rmol[I1236, 12, 36]
plotfit[freqs1236, I1236];
```

3.53301×10^{-46}

1.53779×10^{-10}



Finally, we compare the moments of inertia and interatomic distances for the different isotopes:

```
(I1234 - I1232) / I1232
(I1236 - I1234) / I1232
```

0.0160826

0.0149067

```
(R1234 - R1232) / R1232
(R1236 - R1234) / R1232
```

-0.000109108

-0.0000172965

As expected, the moment of inertia increases linearly with small changes in sulfur mass ($\sim 0.75\,\%/1\,\text{amu}$), and so the spectrum scales tighter as seen in the plots. However, the interatomic distances are roughly the same, which is also expected since the physics of molecular bonding is hardly affected by nuclear mass at low rotation and vibration levels.