

HW #9

1. A=210

These nuclides add two nucleons to the double-magic ^{208}Pb . For ^{210}Pb , we add two neutrons into the $2g_{9/2}$ orbital. Taking the proper anti-symmetry of two neutrons into account, the possible spin-parities are $0^+, 2^+, 4^+, 6^+, 8^+$. The lower J give lower energy because the overlap of the spatial wave functions between two neutrons is greater and hence the attractive potential brings the energy down; the opposite of the Hund's rule in atoms that try to separate the spatial wave functions due to the Coulomb *repulsion*. (It is not clear what the next 10^+ state is; being in parenthesis means it is not well-established either.)

Similarly for ^{210}Po , we add two protons into the $1h_{9/2}$ orbital. Again due to the anti-symmetry, the possible spin-parities are $0^+, 2^+, 4^+, 6^+, 8^+$. Again the attractive nuclear force orders these states from the lowest to the highest energy.

^{210}Bi is interesting. Because we add one neutron in $2g_{9/2}$ and one proton in $1h_{9/2}$ orbital, the parity is odd $(-1)^4 (-1)^5 = -1$. The total angular momentum ranges all the way from 0 to 9, because there is no anti-symmetry requirement between the proton and the neutron. Indeed, we find states $1^-, 0^-, 9^-, 2^-, 3^-, 7^-, 5^-, 4^-, 6^-$, and 8^- (skipping the not-yet-established 1^- state which is presumably due to a different shell-model configuration). Understanding their ordering is not trivial, but it is easy to see that the ordering is sensitive to the details of the attractive force between the proton and the neutron and their wavefunctions. For the sake of discussions, imagine an *attractive* Coulomb potential as a model of interaction between them. Then the expectation value of the interaction potential can be calculated the same way you worked out the Coulomb energies in $n p^2$ configuration in the midterm exam by expanding the Coulomb potential in multipoles. In our case, putting g ($l = 4$) and h ($l = 5$) together, multipoles of $\lambda = 1, 2, 3, 4, 5, 6, 7, 8, 9$ would contribute, each term with a different radial integral. Given the linear combination of nine terms, any ordering among ten states is possible.

2. A=17

These nuclides add one nucleon to the double-magic ^{16}O . Looking at the energy levels, they all appear as $I = 1/2$ doublets at least up to $5/2^+$ (6862 keV for oxygen and 6697 keV for fluorine).

The ground state $5/2^+$ is understood by simply putting the nucleon in the $1d_{5/2}$ orbital.

The first excited state $1/2^+$ is understood by simply putting the nucleon in the $2s_{1/2}$ orbital.

The second ($1/2^-$), third ($5/2^-$), and fourth ($3/2^-$) excited states have negative parity, indicating the role of an odd- l orbital. By exciting one of the nucleons in the closed-shell $1p_{1/2}$ to $1d_{5/2}$, we have one hole in $1p_{1/2}$, and two nucleons in $1d_{5/2}$. There are two possibilities of isospin for two nucleons in $1d_{5/2}$. If $I = 0$, the isospin wave function is anti-symmetric, and the orbit/spin wave functions must be symmetric, allowing for $J = 1, 3$. If $I = 1$, the isospin wave function is symmetric, and the orbit/spin wave functions must be anti-symmetric, allowing for $J = 0, 2$. Further combining with the hole in $1p_{1/2}$, the former gives $1/2^-, 3/2^-, 5/2^-, 7/2^-$, while the latter $1/2^-, 3/2^-, 5/2^-$. Clearly the latter choice matches the data better.

The fifth excited state $3/2^+$ is understood by simply putting the nucleon in the $2d_{3/2}$ orbital.

I stop here.

3. hybrid orbitals

(a) p_x, p_y orbitals

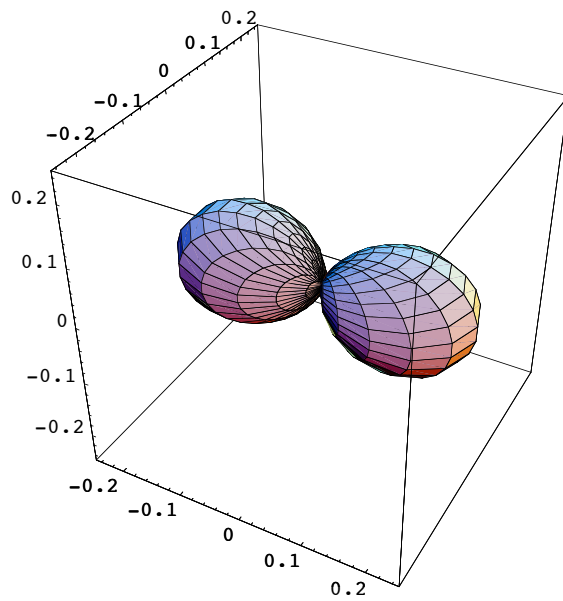
p_x and p_y orbitals are given by the linear combinations of Y_1^1 and Y_1^{-1} . As we did in 221A, we plot the "shape" by plotting the probability as the distance from the origin.

p_x orbital is obtained by

$$\mathbf{p}_x = \text{Simplify}\left[\text{ExpToTrig}\left[-\frac{1}{\sqrt{2}}\left(\text{SphericalHarmonicY}[1, 1, \theta, \phi] - \text{SphericalHarmonicY}[1, -1, \theta, \phi]\right)\right]\right]$$

$$\frac{1}{2} \sqrt{\frac{3}{\pi}} \cos[\phi] \sin[\theta]$$

```
ParametricPlot3D[Abs[px]2 {Sin[θ] Cos[φ], Sin[θ] Sin[φ], Cos[θ]}, {θ, 0, π},
{φ, 0, 2 π}, PlotRange → {{-0.25, 0.25}, {-0.25, 0.25}, {-0.25, 0.25}}]
```

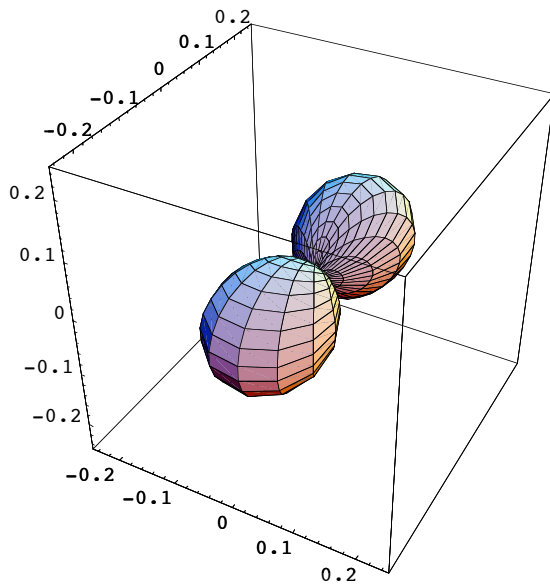


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```
py = Simplify[
  ExpToTrig[ $\frac{1}{\sqrt{2}}$  (SphericalHarmonicY[1, 1, θ, φ] + SphericalHarmonicY[1, -1, θ, φ])] ]
```

$$\frac{1}{2} \sqrt{\frac{3}{\pi}} \sin[\theta] \sin[\phi]$$

```
ParametricPlot3D[Abs[py]2 {Sin[θ] Cos[φ], Sin[θ] Sin[φ], Cos[θ]}, {θ, 0, π},
{φ, 0, 2 π}, PlotRange → {{-0.25, 0.25}, {-0.25, 0.25}, {-0.25, 0.25}}]
```



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(b) $s p^2$ orbitals

We take three independent linear combinations of s , p_x , and p_y orbitals. Because the orbital wave functions are different for them, this is a tricky question. If we plot the probability on the angles integrated over the entire radii appears as the relative weight between the s and the p orbitals. For the graphical representations, we choose the relative weight to be one.

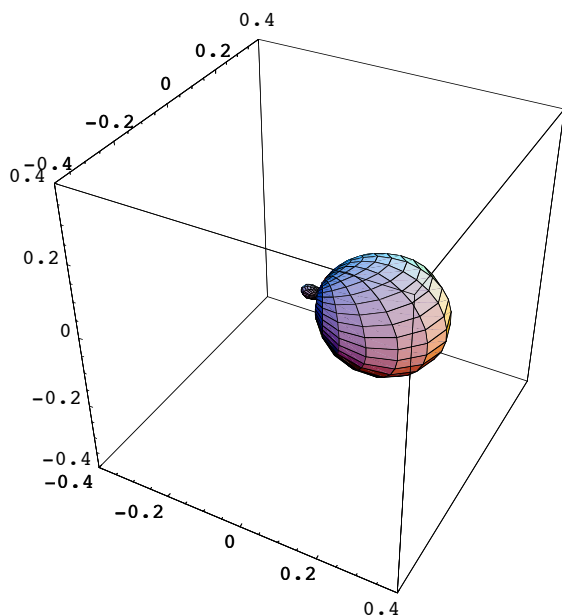
The three orthonormal linear combinations are

$$\begin{aligned} \frac{1}{\sqrt{3}} s + \sqrt{\frac{2}{3}} p_x \\ \frac{1}{\sqrt{3}} s - \sqrt{\frac{1}{6}} p_x + \frac{1}{\sqrt{2}} p_y \\ \frac{1}{\sqrt{3}} s - \sqrt{\frac{1}{6}} p_x - \frac{1}{\sqrt{2}} p_y \end{aligned}$$

s = SphericalHarmonicY[0, 0, θ, φ]

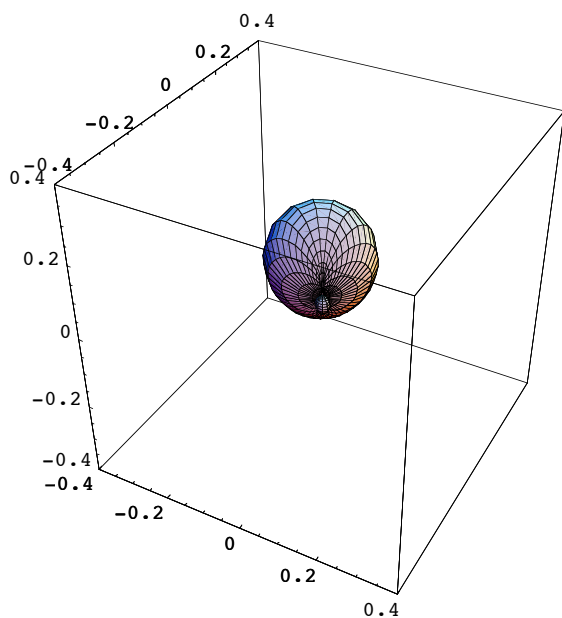
$$\frac{1}{2\sqrt{\pi}}$$

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ParametricPlot3D[Abs[ $\frac{1}{\sqrt{3}} s + \sqrt{\frac{2}{3}} p_x$ ]^2 {Sin[ $\theta$ ] Cos[ $\phi$ ], Sin[ $\theta$ ] Sin[ $\phi$ ], Cos[ $\theta$ ]},
{ $\theta$ , 0,  $\pi$ }, { $\phi$ , 0,  $2\pi$ }, PlotRange -> {{-0.4, 0.4}, {-0.4, 0.4}, {-0.4, 0.4}}
```



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```
ParametricPlot3D[Abs[ $\frac{1}{\sqrt{3}} s - \sqrt{\frac{1}{6}} p_x + \frac{1}{\sqrt{2}} p_y$ ]^2 {Sin[ $\theta$ ] Cos[ $\phi$ ], Sin[ $\theta$ ] Sin[ $\phi$ ], Cos[ $\theta$ ]},
{ $\theta$ , 0,  $\pi$ }, { $\phi$ , 0,  $2\pi$ }, PlotRange -> {{-0.4, 0.4}, {-0.4, 0.4}, {-0.4, 0.4}}
```

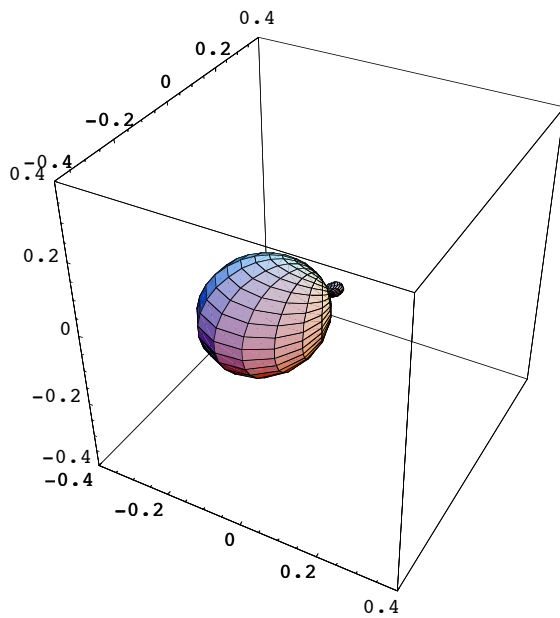


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ParametricPlot3D[Abs[ $\frac{1}{\sqrt{3}} s - \sqrt{\frac{1}{6}} p_x - \frac{1}{\sqrt{2}} p_y$ ]2 {Sin[ $\theta$ ] Cos[ $\phi$ ], Sin[ $\theta$ ] Sin[ $\phi$ ], Cos[ $\theta$ ]},
{ $\theta$ , 0,  $\pi$ }, { $\phi$ , 0,  $2\pi$ }, PlotRange -> {{-0.4, 0.4}, {-0.4, 0.4}, {-0.4, 0.4}}]

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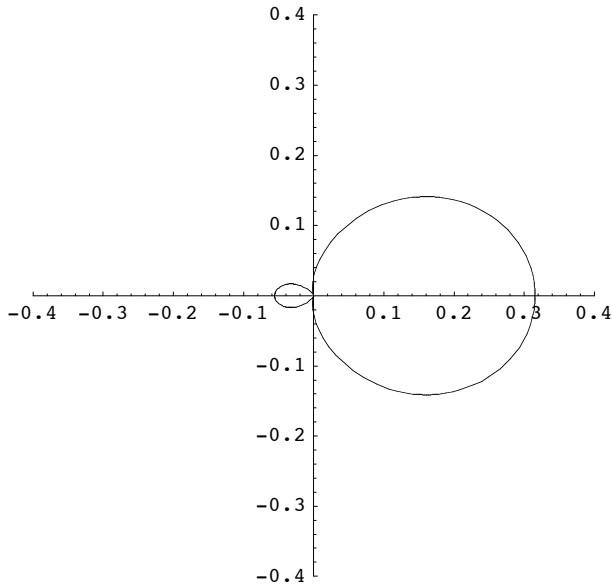
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All of them are more or less along the $x - y$ plane. It is more instructive to look at the slice on the $x - y$ plane,

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ParametricPlot[Abs[ $\frac{1}{\sqrt{3}} s + \sqrt{\frac{2}{3}} p_x$ ]2 {Sin[ $\theta$ ] Cos[ $\phi$ ], Sin[ $\theta$ ] Sin[ $\phi$ ]} /. { $\theta \rightarrow \frac{\pi}{2}$ },
{ $\phi, 0, 2 \pi$ }, PlotRange -> {{-0.4, 0.4}, {-0.4, 0.4}}, AspectRatio -> 1]

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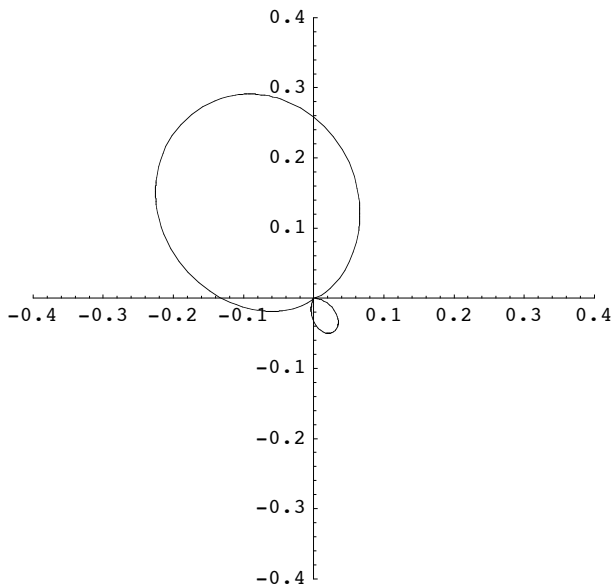


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ParametricPlot[Abs[ $\frac{1}{\sqrt{3}} s - \sqrt{\frac{1}{6}} p_x + \frac{1}{\sqrt{2}} p_y$ ]2 {Sin[ $\theta$ ] Cos[ $\phi$ ], Sin[ $\theta$ ] Sin[ $\phi$ ]} /. { $\theta \rightarrow \frac{\pi}{2}$ },
{ $\phi, 0, 2 \pi$ }, PlotRange -> {{-0.4, 0.4}, {-0.4, 0.4}}, AspectRatio -> 1]

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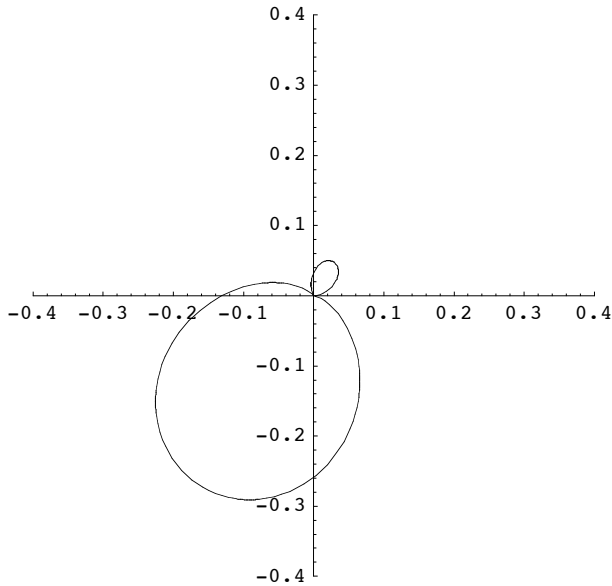


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ParametricPlot[Abs[ $\frac{1}{\sqrt{3}} s - \sqrt{\frac{1}{6}} p_x - \frac{1}{\sqrt{2}} p_y$ ]2 {Sin[ $\theta$ ] Cos[ $\phi$ ], Sin[ $\theta$ ] Sin[ $\phi$ ]} /. { $\theta \rightarrow \frac{\pi}{2}$ },
{ $\phi$ , 0, 2  $\pi$ }, PlotRange -> {{-0.4, 0.4}, {-0.4, 0.4}}, AspectRatio -> 1]

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- Graphics -

Therefore these orbitals "stick out" to directions 120 degrees from each other.

(c) $s p^3$ orbitals

We take three independent linear combinations of s , p_x , p_y , and p_z orbitals. Because the orbital wave functions are different for them, this is a tricky question. If we plot the probability on the angles integrated over the entire radii appears as the relative weight between the s and the p orbitals. For the graphical representations, we choose the relative weight to be one.

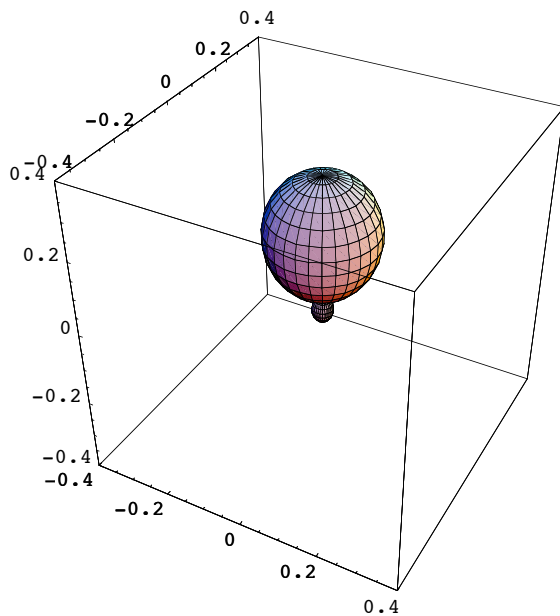
The four orthonormal linear combinations are

$$\begin{aligned} & \frac{1}{2} s + \frac{\sqrt{3}}{2} p_z \\ & \frac{1}{2} s - \frac{1}{2\sqrt{3}} p_z + \sqrt{\frac{2}{3}} p_x \\ & \frac{1}{2} s - \frac{1}{2\sqrt{3}} p_z - \frac{1}{\sqrt{6}} p_x + \frac{1}{\sqrt{2}} p_y \\ & \frac{1}{2} s - \frac{1}{2\sqrt{3}} p_z - \frac{1}{\sqrt{6}} p_x - \frac{1}{\sqrt{2}} p_y \end{aligned}$$

$p_z = \text{SphericalHarmonicY}[1, 0, \theta, \phi]$

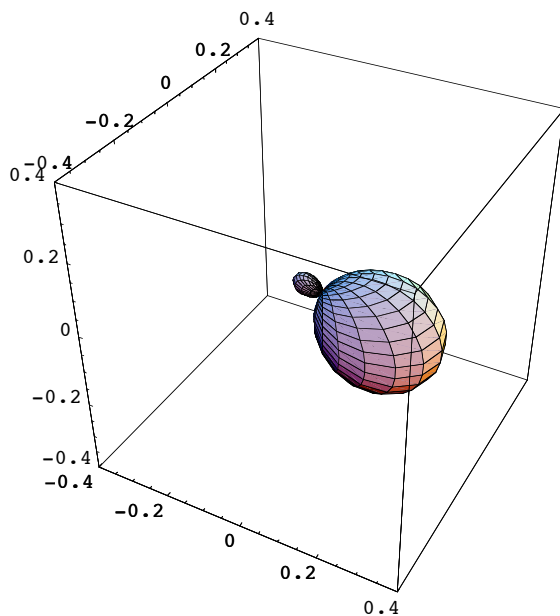
$$\frac{1}{2} \sqrt{\frac{3}{\pi}} \text{Cos}[\theta]$$


```
ParametricPlot3D[Abs[ $\frac{1}{2} s + \frac{\sqrt{3}}{2} p_z$ ]  $\{ \text{Sin}[\theta] \text{Cos}[\phi], \text{Sin}[\theta] \text{Sin}[\phi], \text{Cos}[\theta] \}$ ,
{ $\theta, 0, \pi$ }, { $\phi, 0, 2\pi$ }, PlotRange  $\rightarrow \{ \{-0.4, 0.4\}, \{-0.4, 0.4\}, \{-0.4, 0.4\} \}$ ]
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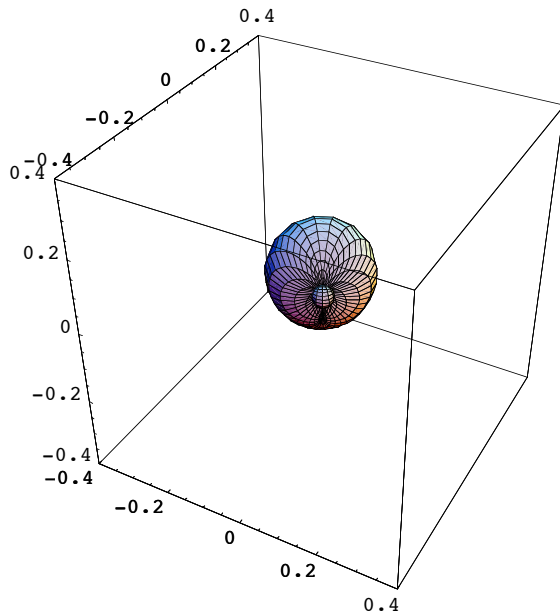
- Graphics3D -

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ParametricPlot3D[Abs[ $\frac{1}{2} s - \frac{1}{2\sqrt{3}} p_z + \sqrt{\frac{2}{3}} p_x$ ]  $\{ \text{Sin}[\theta] \text{Cos}[\phi], \text{Sin}[\theta] \text{Sin}[\phi], \text{Cos}[\theta] \}$ ,
{ $\theta, 0, \pi$ }, { $\phi, 0, 2\pi$ }, PlotRange  $\rightarrow \{ \{-0.4, 0.4\}, \{-0.4, 0.4\}, \{-0.4, 0.4\} \}$ ]
```



- Graphics3D -

```
ParametricPlot3D[  
  Abs[ $\frac{1}{2} s - \frac{1}{2\sqrt{3}} p_z - \frac{1}{\sqrt{6}} p_x + \frac{1}{\sqrt{2}} p_y$ ]2 {Sin[ $\theta$ ] Cos[ $\phi$ ], Sin[ $\theta$ ] Sin[ $\phi$ ], Cos[ $\theta$ ]},  
  { $\theta$ , 0,  $\pi$ }, { $\phi$ , 0,  $2\pi$ }, PlotRange -> {{-0.4, 0.4}, {-0.4, 0.4}, {-0.4, 0.4}}
```

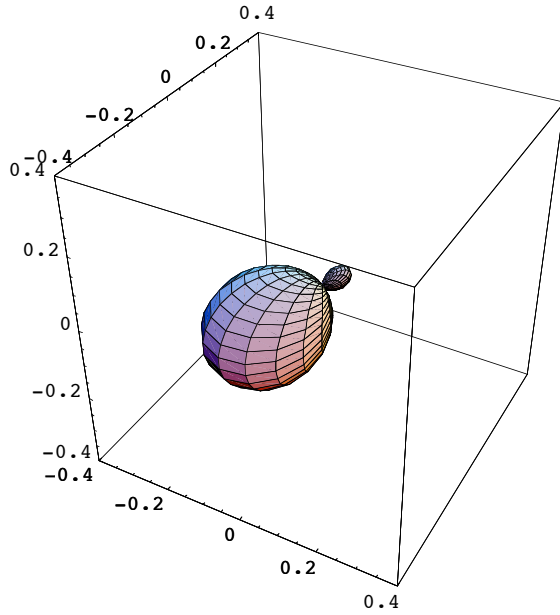


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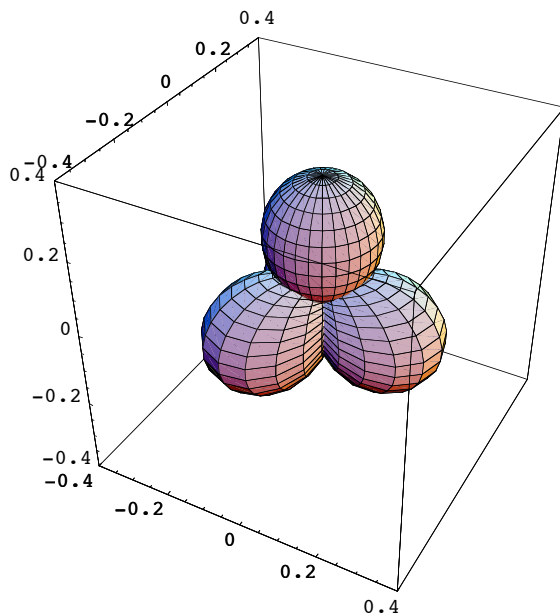
ParametricPlot3D[
  Abs[ $\frac{1}{2} s - \frac{1}{2\sqrt{3}} p_z - \frac{1}{\sqrt{6}} p_x - \frac{1}{\sqrt{2}} p_y$ ]2 {Sin[ $\theta$ ] Cos[ $\phi$ ], Sin[ $\theta$ ] Sin[ $\phi$ ], Cos[ $\theta$ ]},
  { $\theta$ , 0,  $\pi$ }, { $\phi$ , 0,  $2\pi$ }, PlotRange -> {{-0.4, 0.4}, {-0.4, 0.4}, {-0.4, 0.4}}]

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- Graphics3D -

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Show[%, %, %%, %%%]
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- Graphics3D -

They form a tetrahedral shape.

4. Harmonic Oscillator

(a)

$p = \partial L / \partial \dot{x} = m \dot{x}$. Therefore, $L = p \dot{x} - \frac{p^2}{2m} - \frac{1}{2} m \omega^2 x^2$, which is consistent with the general form $L = p \dot{q} - H(p, q)$.

(b)

Using $x = \sqrt{\frac{\hbar}{2m\omega}} (a + a^\dagger)$, $p = -i \sqrt{\frac{m\hbar\omega}{2}} (a - a^\dagger)$, we find

$$p \dot{x} = -i \sqrt{\frac{m\hbar\omega}{2}} (a - a^\dagger) \sqrt{\frac{\hbar}{2m\omega}} (\dot{a} + \dot{a}^\dagger) = -i \frac{\hbar}{2} (a \dot{a} + a \dot{a}^\dagger - a^\dagger \dot{a} - a^\dagger \dot{a}^\dagger).$$

The first and the last terms are total derivatives, and can be dropped from the Lagrangian. Integrating the second terms in parts, we find $p \dot{x} = i \hbar a^\dagger \dot{a}$ up to surface terms. The Hamiltonian is

$$\frac{p^2}{2m} + \frac{1}{2} m \omega^2 x^2 = -\frac{\hbar\omega}{4} (a - a^\dagger)^2 + \frac{\hbar\omega}{4} (a + a^\dagger)^2 = \frac{\hbar\omega}{2} (a a^\dagger + a^\dagger a) = \hbar\omega (a^\dagger a + \frac{1}{2}).$$

Therefore,

$$L = i \hbar a^\dagger \dot{a} - \hbar\omega (a^\dagger a + \frac{1}{2}).$$

(c)

Because of the form of the Lagrangian, we can identify a as the canonical coordinate, while $\partial L / \partial \dot{a} = i \hbar a^\dagger$ is its canonically conjugate momentum. Therefore, the canonical commutation relation would be $[a, i \hbar a^\dagger] = i \hbar$, and hence $[a, a^\dagger] = 1$. The Hamiltonian is nothing but $H = \hbar\omega (a^\dagger a + \frac{1}{2})$.

This is just a confirmation that the analytical mechanics is so versatile that you can choose whatever you want for the canonical coordinates.

(d)

The Hamiltonian is $H = \frac{\hbar\omega}{2} (a a^\dagger + a^\dagger a) = \hbar\omega (a^\dagger a - \frac{1}{2})$. Namely, the zero-point energy is *negative*, unlike the usual (bosonic) harmonic oscillator.

The ground state is given by $a |0\rangle = 0$ as usual. Its energy eigenvalue is $H |0\rangle = \frac{-1}{2} \hbar\omega |0\rangle$.

The excited state is given by $|1\rangle = a^\dagger |0\rangle$. Its energy eigenvalue is

$$\begin{aligned} H |1\rangle &= \hbar\omega (a^\dagger a - \frac{1}{2}) a^\dagger |0\rangle = \hbar\omega (a^\dagger a a^\dagger - \frac{1}{2} a^\dagger) |0\rangle \\ &= \hbar\omega (a^\dagger (-a^\dagger a + 1) - \frac{1}{2} a^\dagger) |0\rangle = \hbar\omega \frac{1}{2} a^\dagger |0\rangle = \frac{1}{2} \hbar\omega |1\rangle \end{aligned}$$

Therefore, its energy eigenvalue is $\frac{1}{2} \hbar\omega$.

Using the anti-commutation relation $\{a^\dagger, a^\dagger\} = 2(a^\dagger)^2 = 0$, acting a^\dagger twice on the ground state returns zero. Therefore, the Hilbert space consists of only two states, $|0\rangle$ and $|1\rangle$.