

Solutions of Homework #5

Problem 1

10.15 The state $|\psi_{-}\rangle$ is

$$|\psi_{-}\rangle = \frac{1}{\sqrt{2}}(|200\rangle + |210\rangle)$$

The expectation value of the dipole moment $\mathbf{d} = -e\mathbf{r}$ is

$$\begin{aligned} \langle \psi_{-} | \mathbf{d} | \psi_{-} \rangle &= \langle \psi_{-} | -e\mathbf{r} | \psi_{-} \rangle = -e \frac{1}{\sqrt{2}} (\langle 200 | + \langle 210 |) \mathbf{r} \frac{1}{\sqrt{2}} (|200\rangle + |210\rangle) \\ &= -e \frac{1}{2} (\langle 200 | \mathbf{r} | 200 \rangle + \langle 200 | \mathbf{r} | 210 \rangle + \langle 210 | \mathbf{r} | 200 \rangle + \langle 210 | \mathbf{r} | 210 \rangle) \end{aligned}$$

The first and last terms are zero by symmetry and the other two terms are complex conjugates of each other. Hence we need to find

$$\begin{aligned} \langle 200 | \mathbf{r} | 210 \rangle &= \int \psi_{200}^{(0)*}(r, \theta, \phi) (x\hat{\mathbf{i}} + y\hat{\mathbf{j}} + z\hat{\mathbf{k}}) \psi_{210}^{(0)}(r, \theta, \phi) r^2 \sin\theta dr d\theta d\phi \\ &= \frac{2}{(2a_0)^{3/2}} \frac{1}{\sqrt{4\pi}} \frac{1}{\sqrt{3}a_0(2a_0)^{3/2}} \sqrt{\frac{3}{4\pi}} \int_0^\infty r \left(1 - \frac{r}{2a_0}\right) e^{-r/a_0} (x\hat{\mathbf{i}} + y\hat{\mathbf{j}} + z\hat{\mathbf{k}}) r^2 dr \\ &\quad \int_0^\pi \cos\theta \sin\theta d\theta \int_0^{2\pi} d\phi \\ &= \frac{1}{16\pi a_0^4} \int_0^\infty \int_0^{2\pi} \int_0^\pi r^4 \left(1 - \frac{r}{2a_0}\right) e^{-r/a_0} (\sin\theta \cos\theta \hat{\mathbf{i}} + \sin\theta \sin\theta \hat{\mathbf{j}} + \cos\theta \hat{\mathbf{k}}) \cos\theta \sin\theta d\theta d\phi dr \end{aligned}$$

The azimuthal integrals $\int_0^{2\pi} \cos\phi d\phi$ and $\int_0^{2\pi} \sin\phi d\phi$ are both zero. The remaining polar integral gives 2/3, yielding

$$\begin{aligned} \langle 200 | \mathbf{r} | 210 \rangle &= \frac{\hat{\mathbf{k}}}{16\pi a_0^4} \frac{2}{3} 2\pi \int_0^\infty r^4 \left(1 - \frac{r}{2a_0}\right) e^{-r/a_0} dr \\ &= \frac{\hat{\mathbf{k}}}{12a_0^4} \left[\int_0^\infty r^4 e^{-r/a_0} dr - \frac{1}{2a_0} \int_0^\infty r^5 e^{-r/a_0} dr \right] = \frac{\hat{\mathbf{k}}}{12a_0^4} \left[4!a_0^5 - \frac{1}{2a_0} 5!a_0^6 \right] \\ &= -3a_0 \hat{\mathbf{k}} \end{aligned}$$

The expectation value of the dipole moment is

$$\begin{aligned} \langle \psi_{-} | \mathbf{d} | \psi_{-} \rangle &= -e \frac{1}{2} (\langle 200 | \mathbf{r} | 210 \rangle + \langle 210 | \mathbf{r} | 200 \rangle) \\ &= -e \frac{1}{2} (-3a_0 \hat{\mathbf{k}} + -3a_0 \hat{\mathbf{k}}) \\ &= 3ea_0 \hat{\mathbf{k}} \end{aligned}$$

which means it is aligned with the applied electric field, as expected [see Fig. 8.9(b)].

Problem 2

10.23 a) For the unperturbed case ($\varepsilon = 0$) we have

$$H_0 \doteq V_0 \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 4 \end{pmatrix}$$

with eigenvalues $E_1 = V_0$, $E_2 = V_0$, $E_3 = 4V_0$ and eigenvectors

$$|1\rangle \doteq \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \quad |2\rangle \doteq \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \quad |3\rangle \doteq \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$$

Note that $|1\rangle$ and $|2\rangle$ are degenerate and $|3\rangle$ is nondegenerate.

b) Now look at the perturbation of the nondegenerate $|3\rangle$ state. First we need to write the perturbation Hamiltonian $H' = H - H_0$

$$H' \doteq V_0 \begin{pmatrix} 0 & 2\varepsilon & 0 \\ 2\varepsilon & 0 & 3\varepsilon \\ 0 & 3\varepsilon & 0 \end{pmatrix}$$

The first-order energy correction is

$$E_n^{(1)} = \langle n^{(0)} | H' | n^{(0)} \rangle$$

$$E_3^{(1)} = \langle 3^{(0)} | H' | 3^{(0)} \rangle = 0$$

$$\boxed{E_3^{(1)} = 0}$$

The second-order energy correction is

$$E_3^{(2)} = \sum_{k \neq 3} \frac{|\langle 3^{(0)} | H' | k^{(0)} \rangle|^2}{E_3^{(0)} - E_k^{(0)}} = \frac{|\langle 3^{(0)} | H' | 1^{(0)} \rangle|^2}{E_3^{(0)} - E_1^{(0)}} + \frac{|\langle 3^{(0)} | H' | 2^{(0)} \rangle|^2}{E_3^{(0)} - E_2^{(0)}}$$

$$= \frac{|0|^2}{4V_0 - V_0} + \frac{|3\varepsilon V_0|^2}{4V_0 - V_0} = 3\varepsilon^2 V_0$$

Hence the corrected energy is

$$E_3 = E_3^{(0)} + E_3^{(1)} + E_3^{(2)} = 4V_0 + 0 + 3\varepsilon^2 V_0$$

$$\boxed{E_3 = V_0 [4 + 3\varepsilon^2]}$$

c) Now look at the perturbation of the degenerate $|1\rangle$ and $|2\rangle$ states. Here we need to diagonalize the perturbation Hamiltonian within that 2x2 space:

$$H' \doteq V_0 \begin{pmatrix} 0 & 2\varepsilon & 0 \\ 2\varepsilon & 0 & 3\varepsilon \\ 0 & 3\varepsilon & 0 \end{pmatrix} \Rightarrow H'_{1,2} \doteq V_0 \begin{pmatrix} 0 & 2\varepsilon \\ 2\varepsilon & 0 \end{pmatrix}$$

Diagonalizing gives

$$\begin{vmatrix} -\lambda & 2\varepsilon V_0 \\ 2\varepsilon V_0 & -\lambda \end{vmatrix} = 0$$

$$(-\lambda)(-\lambda) - (2\varepsilon V_0)^2 = 0$$

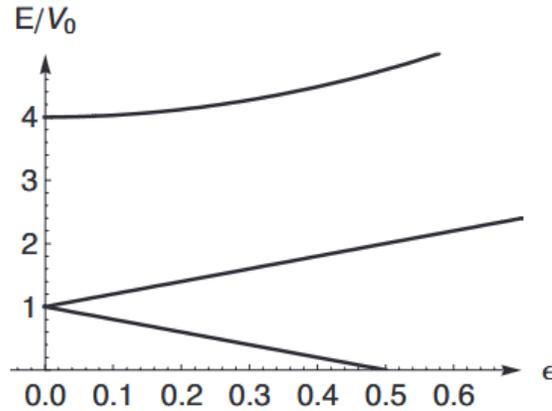
$$(\lambda^2 - 4\varepsilon^2 V_0^2) = 0$$

$$\lambda = \pm 2\varepsilon V_0$$

$$\boxed{E_1 = E_1^{(0)} + E_1^{(1)} = V_0 + 2\varepsilon V_0 = V_0(1 + 2\varepsilon)}$$

$$\boxed{E_2 = E_2^{(0)} + E_2^{(1)} = V_0 - 2\varepsilon V_0 = V_0(1 - 2\varepsilon)}$$

d) The degenerate levels split linearly, while the nondegenerate level has a quadratic dependence and is repelled by the one lower level it is coupled to, as expected.



Problem 3

10.24

$$H \doteq V_0 \begin{pmatrix} 3 & \epsilon & 0 & 0 \\ \epsilon & 3 & 2\epsilon & 0 \\ 0 & 2\epsilon & 5 & \epsilon \\ 0 & 0 & \epsilon & 7 \end{pmatrix}$$

a) For the unperturbed case we have

$$H_0 \doteq V_0 \begin{pmatrix} 3 & 0 & 0 & 0 \\ 0 & 3 & 0 & 0 \\ 0 & 0 & 5 & 0 \\ 0 & 0 & 0 & 7 \end{pmatrix}$$

with eigenvalues $E_1 = 3V_0, E_2 = 3V_0, E_3 = 5V_0, E_4 = 7V_0$ and eigenvectors

$$|1\rangle \doteq \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}, |2\rangle \doteq \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}, |3\rangle \doteq \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix}, |4\rangle \doteq \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}$$

Note that $|1\rangle$ and $|2\rangle$ are degenerate and $|3\rangle$ and $|4\rangle$ are nondegenerate.

b) Let's first do nondegenerate perturbation theory for the $|3\rangle$ and $|4\rangle$ states. First we need to write the perturbation Hamiltonian:

$$H' \doteq V_0 \begin{pmatrix} 0 & \epsilon & 0 & 0 \\ \epsilon & 0 & 2\epsilon & 0 \\ 0 & 2\epsilon & 0 & \epsilon \\ 0 & 0 & \epsilon & 0 \end{pmatrix}$$

The first-order corrections are

$$E_n^{(1)} = \langle n^{(0)} | \hat{H}' | n^{(0)} \rangle$$

$$E_3^{(1)} = \langle 3^{(0)} | \hat{H}' | 3^{(0)} \rangle = 0$$

$$E_4^{(1)} = \langle 4^{(0)} | \hat{H}' | 4^{(0)} \rangle = 0$$

So we need to go to second order for these states

$$E_n^{(2)} = \sum_{k \neq n} \frac{|\langle n^{(0)} | \hat{H}' | k^{(0)} \rangle|^2}{E_n^{(0)} - E_k^{(0)}}$$

$$E_3^{(2)} = \sum_{k \neq 3} \frac{|\langle 3^{(0)} | \hat{H}' | k^{(0)} \rangle|^2}{E_3^{(0)} - E_k^{(0)}} = \frac{|\langle 3^{(0)} | \hat{H}' | 1^{(0)} \rangle|^2}{E_3^{(0)} - E_1^{(0)}} + \frac{|\langle 3^{(0)} | \hat{H}' | 2^{(0)} \rangle|^2}{E_3^{(0)} - E_2^{(0)}} + \frac{|\langle 3^{(0)} | \hat{H}' | 4^{(0)} \rangle|^2}{E_3^{(0)} - E_4^{(0)}}$$

$$= \frac{|0|^2}{5V_0 - 3V_0} + \frac{|2\varepsilon V_0|^2}{5V_0 - 3V_0} + \frac{|\varepsilon V_0|^2}{5V_0 - 7V_0} = \varepsilon^2 V_0 \left(\frac{4}{2} + \frac{1}{-2} \right) = \frac{3}{2} \varepsilon^2 V_0$$

$$E_4^{(2)} = \sum_{k \neq 4} \frac{|\langle 4^{(0)} | \hat{H}' | k^{(0)} \rangle|^2}{E_4^{(0)} - E_k^{(0)}} = \frac{|\langle 4^{(0)} | \hat{H}' | 1^{(0)} \rangle|^2}{E_4^{(0)} - E_1^{(0)}} + \frac{|\langle 4^{(0)} | \hat{H}' | 2^{(0)} \rangle|^2}{E_4^{(0)} - E_2^{(0)}} + \frac{|\langle 4^{(0)} | \hat{H}' | 3^{(0)} \rangle|^2}{E_4^{(0)} - E_3^{(0)}}$$

$$= \frac{|0|^2}{7V_0 - 3V_0} + \frac{|0|^2}{7V_0 - 3V_0} + \frac{|\varepsilon V_0|^2}{7V_0 - 5V_0} = \frac{1}{2} \varepsilon^2 V_0$$

Thus the energies to second order are

$$E_3 = V_0 \left[5 + \frac{3}{2} \varepsilon^2 \right]$$

$$E_4 = V_0 \left[7 + \frac{1}{2} \varepsilon^2 \right]$$

Now look at the perturbation of the degenerate $|1\rangle$ and $|2\rangle$ states. Here we need to diagonalize the perturbation Hamiltonian within that 2x2 space:

$$H' \doteq V_0 \begin{pmatrix} 0 & \varepsilon & 0 & 0 \\ \varepsilon & 0 & 2\varepsilon & 0 \\ 0 & 2\varepsilon & 0 & \varepsilon \\ 0 & 0 & \varepsilon & 0 \end{pmatrix} \Rightarrow H'_{1,2} \doteq V_0 \begin{pmatrix} 0 & \varepsilon \\ \varepsilon & 0 \end{pmatrix}$$

Diagonalize this

$$\begin{vmatrix} -\lambda & \epsilon V_0 \\ \epsilon V_0 & -\lambda \end{vmatrix} = 0$$

$$\lambda^2 - (\epsilon V_0)^2 = 0$$

$$\lambda = \pm \epsilon V_0$$

The corrected energies are

$$\begin{array}{l} E_1 = E_1^{(0)} + E_1^{(1)} = 3V_0 + \epsilon V_0 \\ E_2 = E_2^{(0)} + E_2^{(1)} = 3V_0 - \epsilon V_0 \end{array}$$

Problem 4

(a)

11.9 Recall the angular momentum commutation relations

$$\begin{aligned} [J_x, J_y] &= i\hbar J_z ; & [J_y, J_z] &= i\hbar J_x ; & [J_z, J_x] &= i\hbar J_y \\ [\mathbf{J}^2, J_x] &= [\mathbf{J}^2, J_y] = [\mathbf{J}^2, J_z] = 0 \end{aligned}$$

Taking commutators with the hyperfine Hamiltonian gives (recall that the electron and proton spin operators commute)

$$\begin{aligned} [H'_{hf}, \mathbf{S}^2] &= \left[\frac{A}{\hbar^2} \mathbf{S} \cdot \mathbf{I}, \mathbf{S}^2 \right] = \frac{A}{\hbar^2} \mathbf{I} \cdot [\mathbf{S}, \mathbf{S}^2] = \frac{A}{\hbar^2} \mathbf{I} \cdot [S_x \mathbf{i} + S_y \mathbf{j} + S_z \mathbf{k}, \mathbf{S}^2] = \\ &= \frac{A}{\hbar^2} \mathbf{I} \cdot \{ \mathbf{i} [S_x, \mathbf{S}^2] + \mathbf{j} [S_y, \mathbf{S}^2] + \mathbf{k} [S_z, \mathbf{S}^2] \} = 0 \\ [H'_{hf}, \mathbf{I}^2] &= \left[\frac{A}{\hbar^2} \mathbf{S} \cdot \mathbf{I}, \mathbf{I}^2 \right] = \frac{A}{\hbar^2} \mathbf{S} \cdot [\mathbf{I}, \mathbf{I}^2] = \frac{A}{\hbar^2} \mathbf{S} \cdot [I_x \mathbf{i} + I_y \mathbf{j} + I_z \mathbf{k}, \mathbf{I}^2] = \\ &= \frac{A}{\hbar^2} \mathbf{S} \cdot \{ \mathbf{i} [I_x, \mathbf{I}^2] + \mathbf{j} [I_y, \mathbf{I}^2] + \mathbf{k} [I_z, \mathbf{I}^2] \} = 0 \\ [H'_{hf}, S_z] &= \left[\frac{A}{\hbar^2} \mathbf{S} \cdot \mathbf{I}, S_z \right] = \frac{A}{\hbar^2} [S_x I_x + S_y I_y + S_z I_z, S_z] \\ &= \frac{A}{\hbar^2} \{ I_x [S_x, S_z] + I_y [S_y, S_z] + I_z [S_z, S_z] \} \\ &= \frac{A}{\hbar^2} \{ -i\hbar S_y I_x + i\hbar S_x I_y \} = \frac{-iA}{\hbar} \{ S_y I_x - S_x I_y \} \neq 0 \\ [H'_{hf}, I_z] &= \left[\frac{A}{\hbar^2} \mathbf{S} \cdot \mathbf{I}, I_z \right] = \frac{A}{\hbar^2} [S_x I_x + S_y I_y + S_z I_z, I_z] \\ &= \frac{A}{\hbar^2} \{ S_x [I_x, I_z] + S_y [I_y, I_z] + S_z [I_z, I_z] \} \\ &= \frac{A}{\hbar^2} \{ -i\hbar I_y S_x + i\hbar I_x S_y \} = \frac{-iA}{\hbar} \{ I_y S_x - I_x S_y \} \neq 0 \end{aligned}$$

(b)

11.7 The ladder operators are

$$\begin{aligned}S_+ &= S_x + iS_y & I_+ &= I_x + iI_y \\S_- &= S_x - iS_y & I_- &= I_x - iI_y\end{aligned}$$

Solve these for the Cartesian components:

$$\begin{aligned}S_x &= \frac{1}{2}(S_+ + S_-) & I_x &= \frac{1}{2}(I_+ + I_-) \\S_y &= \frac{-i}{2}(S_+ - S_-) & I_y &= \frac{-i}{2}(I_+ - I_-)\end{aligned}$$

and substitute to get

$$\begin{aligned}\mathbf{S} \cdot \mathbf{I} &= S_x I_x + S_y I_y + S_z I_z = \frac{1}{2}(S_+ + S_-)\frac{1}{2}(I_+ + I_-) + \frac{-i}{2}(S_+ - S_-)\frac{-i}{2}(I_+ - I_-) + S_z I_z \\&= \frac{1}{4}(S_+ I_+ + S_- I_+ + S_+ I_- + S_- I_-) - \frac{1}{4}(S_+ I_+ - S_- I_+ - S_+ I_- + S_- I_-) + S_z I_z \\&= \frac{1}{2}(S_- I_+ + S_+ I_-) + S_z I_z\end{aligned}$$

Problem 5

11.4 a) A spin 3/2 system has s (or j) equal to 3/2 and so has four possible states with m_s (or m_j) equal to +3/2, +1/2, -1/2, and -3/2. The four eigenstates are

$$|sm_s\rangle = \left| \frac{3}{2}, \frac{3}{2} \right\rangle, \left| \frac{3}{2}, \frac{1}{2} \right\rangle, \left| \frac{3}{2}, \frac{-1}{2} \right\rangle, \left| \frac{3}{2}, \frac{-3}{2} \right\rangle$$

The eigenvalue equations are

$$\begin{aligned}\mathbf{S}^2 |sm_s\rangle &= s(s+1)\hbar^2 |sm_s\rangle = \frac{15}{4}\hbar^2 \left| \frac{3}{2}, m_s \right\rangle \\S_z |sm_s\rangle &= m_s \hbar |sm_s\rangle = \begin{cases} \frac{3}{2}\hbar \left| \frac{3}{2}, \frac{3}{2} \right\rangle \\ \frac{1}{2}\hbar \left| \frac{3}{2}, \frac{1}{2} \right\rangle \\ -\frac{1}{2}\hbar \left| \frac{3}{2}, \frac{-1}{2} \right\rangle \\ -\frac{3}{2}\hbar \left| \frac{3}{2}, \frac{-3}{2} \right\rangle \end{cases}\end{aligned}$$

b) The matrices representing \mathbf{S}^2 and S_z are diagonal in their own basis—the $|sm_s\rangle$ basis, with the diagonal eigenvalues from above:

$$\mathbf{S}^2 \doteq \begin{pmatrix} \frac{15}{4}\hbar^2 & 0 & 0 & 0 \\ 0 & \frac{15}{4}\hbar^2 & 0 & 0 \\ 0 & 0 & \frac{15}{4}\hbar^2 & 0 \\ 0 & 0 & 0 & \frac{15}{4}\hbar^2 \end{pmatrix}$$

$$S_z \doteq \begin{pmatrix} \frac{3}{2}\hbar & 0 & 0 & 0 \\ 0 & \frac{1}{2}\hbar & 0 & 0 \\ 0 & 0 & -\frac{1}{2}\hbar & 0 \\ 0 & 0 & 0 & -\frac{3}{2}\hbar \end{pmatrix}$$

c) Generate the matrices representing S_x and S_y by noting that $S_{\pm} = S_x \pm iS_y$, which gives

$$S_x = \frac{1}{2}(S_+ + S_-)$$

$$S_y = \frac{-i}{2}(S_+ - S_-)$$

First generate S_{\pm} using

$$S_{\pm}|sm_s\rangle = \hbar\sqrt{(s(s+1) - m_s(m_s \pm 1))}|s, m_s \pm 1\rangle$$

which gives the matrix elements

$$\begin{aligned} \langle s'm'_s|S_{\pm}|sm_s\rangle &= \langle s'm'_s|\hbar\sqrt{(s(s+1) - m_s(m_s \pm 1))}|s, m_s \pm 1\rangle \\ &= \hbar\sqrt{(s(s+1) - m_s(m_s \pm 1))}\langle s'm'_s|s, m_s \pm 1\rangle \\ &= \hbar\sqrt{(s(s+1) - m_s(m_s \pm 1))}\delta_{s's'}\delta_{m'_s, m_s \pm 1} \end{aligned}$$

Hence

$$S_+ \doteq \begin{pmatrix} 0 & \sqrt{3}\hbar & 0 & 0 \\ 0 & 0 & 2\hbar & 0 \\ 0 & 0 & 0 & \sqrt{3}\hbar \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

$$S_- \doteq \begin{pmatrix} 0 & 0 & 0 & 0 \\ \sqrt{3}\hbar & 0 & 0 & 0 \\ 0 & 2\hbar & 0 & 0 \\ 0 & 0 & \sqrt{3}\hbar & 0 \end{pmatrix}$$

This gives

$$S_x \doteq \frac{\hbar}{2} \begin{pmatrix} 0 & \sqrt{3} & 0 & 0 \\ \sqrt{3} & 0 & 2 & 0 \\ 0 & 2 & 0 & \sqrt{3} \\ 0 & 0 & \sqrt{3} & 0 \end{pmatrix}$$

$$S_y \doteq \frac{\hbar}{2} \begin{pmatrix} 0 & -i\sqrt{3} & 0 & 0 \\ i\sqrt{3} & 0 & -i2 & 0 \\ 0 & i2 & 0 & -i\sqrt{3} \\ 0 & 0 & i\sqrt{3} & 0 \end{pmatrix}$$

d) To find the eigenvalues of S_x , diagonalize the matrix

$$\det(S_x - \lambda \mathbf{I}) = \begin{vmatrix} -\lambda & \sqrt{3}\hbar/2 & 0 & 0 \\ \sqrt{3}\hbar/2 & -\lambda & \hbar & 0 \\ 0 & \hbar & -\lambda & \sqrt{3}\hbar/2 \\ 0 & 0 & \sqrt{3}\hbar/2 & -\lambda \end{vmatrix}$$

$$= -\lambda(-\lambda(\lambda^2 - 3\hbar^2/4) - \hbar(-\lambda\hbar)) - \sqrt{3}\hbar/2(\sqrt{3}\hbar/2(\lambda^2 - 3\hbar^2/4) - \hbar(0))$$

$$= \lambda^2(\lambda^2 - 3\hbar^2/4) - 3\hbar^2/4(\lambda^2 - 3\hbar^2/4) - \lambda^2\hbar^2$$

$$0 = (\lambda^2 - 3\hbar^2/4)^2 - \lambda^2\hbar^2$$

Solve to get

$$\begin{aligned}(\lambda^2 - 3\hbar^2/4) &= \pm\lambda\hbar \\ \lambda^2 \mp \lambda\hbar - 3\hbar^2/4 &= 0 \\ \lambda &= \pm\frac{\hbar}{2} \pm \sqrt{\left(\frac{\hbar}{2}\right)^2 + \frac{3\hbar^2}{4}} = \pm\frac{\hbar}{2} \pm \hbar\end{aligned}$$

Which gives the four values

$$S_x = \frac{3\hbar}{2}, \frac{\hbar}{2}, -\frac{\hbar}{2}, -\frac{3\hbar}{2}$$

as expected.