Problem 1

Construct the density matrix for an electron that is either in the spin up along $\hat{y}$ (with probability 1/5) or in the state spin down along $\hat{y}$ (with probability 4/5). Find $\langle S_z \rangle$ and $\langle S_x \rangle$ for the electron.

spin up along y: $|\uparrow_y\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\ i\end{pmatrix}$, $\langle\uparrow_y| = \frac{1}{\sqrt{2}}(1, -i)$

spin down along y: $|\downarrow_y\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\ -i\end{pmatrix}$, $\langle\downarrow_y| = \frac{1}{\sqrt{2}}(1, i)$

pure state: $|\uparrow_y\rangle\langle\uparrow_y|$, $|\downarrow_y\rangle\langle\downarrow_y|$

so the density operator: $\rho = \sum_i w_i |\psi_i\rangle\langle\psi_i| = \frac{1}{5}\cdot\frac{1}{2}|\uparrow_y\rangle\langle\uparrow_y| + \frac{4}{5}\frac{1}{2}|\downarrow_y\rangle\langle\downarrow_y|$

$$= \frac{1}{10}\begin{pmatrix}1\\ i\end{pmatrix}(1, -i) + \frac{2}{5}\begin{pmatrix}1\\ -i\end{pmatrix}(1, i)$$

$$= \begin{pmatrix}\frac{1}{10} & \frac{-i}{10}\\ \frac{i}{10} & \frac{1}{10}\end{pmatrix} + \begin{pmatrix}\frac{2}{5} & \frac{2}{5}i\\ -\frac{2}{5}i & \frac{2}{5}\end{pmatrix} = \begin{pmatrix}\frac{1}{2} & \frac{3}{10}i\\ -\frac{3}{10}i & \frac{1}{2}\end{pmatrix}$$

Pauli matrix: $\sigma_x = \begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}$, $\sigma_z = \begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}$

spin operator: $S_z = \frac{\hbar}{2}\sigma_z$, $S_x = \frac{\hbar}{2}\sigma_x$

expectation value of an observable S_z and S_x:

$$\langle S_z\rangle = Tr(S_z \rho) = \frac{\hbar}{2} Tr\left(\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}\begin{pmatrix}\frac{1}{2} & \frac{3}{10}i\\ -\frac{3}{10}i & \frac{1}{2}\end{pmatrix}\right) = 0$$

$$\langle S_x\rangle = Tr(S_x \rho) = \frac{\hbar}{2} Tr\left(\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}\begin{pmatrix}\frac{1}{2} & \frac{3}{10}i\\ -\frac{3}{10}i & \frac{1}{2}\end{pmatrix}\right) = 0$$

Problem 2

Take the three-particle fermionic state from HW #2, problem 2(b) and construct the pure state density matrix. Perform a trace over the spin of particle #1 and confirm that the remaining state is antisymmetric under exchange of particle #2 and #3.

$$
\begin{aligned}
|\psi\rangle_{1,2,3} = \frac{1}{\sqrt{6}} \Big\{ & \big[\psi_1(x_1\uparrow)\psi_1(x_2\downarrow)\psi_2(x_3\uparrow) - \psi_1(x_1\downarrow)\psi_1(x_2\uparrow)\psi_2(x_3\uparrow)\big] \\
& + \big[\psi_1(x_2\uparrow)\psi_1(x_3\downarrow)\psi_2(x_1\uparrow) - \psi_1(x_2\downarrow)\psi_1(x_3\uparrow)\psi_2(x_1\uparrow)\big] \\
& - \big[\psi_1(x_1\uparrow)\psi_1(x_3\downarrow)\psi_2(x_2\uparrow) - \psi_1(x_1\downarrow)\psi_1(x_3\uparrow)\psi_2(x_2\uparrow)\big] \Big\}
\end{aligned}
$$

perform a trace over the spin of particle 1:

the density operator:

$$
\begin{aligned}
\rho = |\psi\rangle\langle\psi| = \frac{1}{6} \Big| & \big[\psi_1(x_1\uparrow)\underbrace{\psi_1(x_2\downarrow)\psi_2(x_3\uparrow)}_{1} - \psi_1(x_1\downarrow)\underbrace{\psi_1(x_2\uparrow)\psi_2(x_3\uparrow)}_{10}\big] \\
& + \big[\underbrace{\psi_1(x_2\uparrow)\psi_1(x_3\downarrow)}_{3}\psi_2(x_1\uparrow) - \underbrace{\psi_1(x_2\downarrow)\psi_1(x_3\uparrow)}_{4}\psi_2(x_1\uparrow)\big] \\
& - \big[\psi_1(x_1\uparrow)\underbrace{\psi_1(x_3\downarrow)\psi_2(x_2\uparrow)}_{2} - \psi_1(x_1\downarrow)\underbrace{\psi_1(x_3\uparrow)\psi_2(x_2\uparrow)}_{9}\big] \Big\rangle \\
& \Big\langle \big[\psi_1(x_1\uparrow)\underbrace{\psi_1(x_2\downarrow)\psi_2(x_3\uparrow)}_{5} - \psi_1(x_1\downarrow)\underbrace{\psi_1(x_2\uparrow)\psi_2(x_3\uparrow)}_{12}\big] \\
& + \big[\underbrace{\psi_1(x_2\uparrow)\psi_1(x_3\downarrow)}_{7}\psi_2(x_1\uparrow) - \underbrace{\psi_1(x_2\downarrow)\psi_1(x_3\uparrow)}_{8}\psi_2(x_1\uparrow)\big] \\
& - \big[\psi_1(x_1\uparrow)\underbrace{\psi_1(x_3\downarrow)\psi_2(x_2\uparrow)}_{6} - \psi_1(x_1\downarrow)\underbrace{\psi_1(x_3\uparrow)\psi_2(x_2\uparrow)}_{11}\big] \Big|
\end{aligned}
$$

$$Tr[\rho] = \frac{1}{6}\left[\langle x_1\uparrow|\hat{\rho}|x_1\uparrow\rangle + \langle x_1\downarrow|\hat{\rho}|x_1\downarrow\rangle\right]$$

$$= \frac{1}{6}\Big|\psi_1(x_1)\underbrace{\psi_1(x_2\downarrow)\psi_2(x_3\uparrow)}_{1} - \psi_1(x_1)\underbrace{\psi_2(x_2\uparrow)\psi_1(x_3\downarrow)}_{2}$$

$$+ \psi_2(x_1)\underbrace{\psi_1(x_2\uparrow)\psi_1(x_3\downarrow)}_{3} - \psi_2(x_1)\underbrace{\psi_1(x_2\downarrow)\psi_1(x_3\uparrow)}_{4}\Big\rangle$$

$$\Big\langle\psi_1(x_1)\underbrace{\psi_1(x_2\downarrow)\psi_2(x_3\uparrow)}_{5} - \psi_1(x_1)\underbrace{\psi_2(x_2\uparrow)\psi_1(x_3\downarrow)}_{6}$$

$$+ \psi_2(x_1)\underbrace{\psi_1(x_2\uparrow)\psi_1(x_3\downarrow)}_{7} - \psi_2(x_1)\underbrace{\psi_1(x_2\downarrow)\psi_1(x_3\uparrow)}_{8}\Big|$$

$$+\frac{1}{6}\Big|\psi_1(x_1)\underbrace{\psi_2(x_2\uparrow)\psi_1(x_3\uparrow)}_{9} - \psi_1(x_1)\underbrace{\psi_1(x_2\uparrow)\psi_2(x_3\uparrow)}_{10}\Big\rangle$$

$$\Big\langle\psi_1(x_1)\underbrace{\psi_2(x_2\uparrow)\psi_1(x_3\uparrow)}_{11} - \psi_1(x_1)\underbrace{\psi_1(x_2\uparrow)\psi_2(x_3\uparrow)}_{12}\Big|$$

if we exchange particle 2 and 3 for the 1st pure state:

in part 1: $\psi_1(x_1)\psi_1(x_2\downarrow)\psi_2(x_3\uparrow) \longrightarrow \psi_1(x_1)\psi_1(x_3\downarrow)\psi_2(x_2\uparrow)$

in part 2: $-\psi_1(x_1)\psi_2(x_2\uparrow)\psi_1(x_3\downarrow) \rightarrow -\psi_1(x_1)\psi_2(x_3\uparrow)\psi_1(x_2\downarrow)$

in part 3: $\psi_2(x_1)\psi_1(x_2\uparrow)\psi_1(x_3\downarrow) \rightarrow \psi_2(x_1)\psi_1(x_3\uparrow)\psi_1(x_2\downarrow)$

in part 4: $-\psi_2(x_1)\psi_1(x_2\downarrow)\psi_1(x_3\uparrow) \rightarrow -\psi_2(x_1)\psi_1(x_3\downarrow)\psi_1(x_2\uparrow)$

hence: $$\frac{1}{\sqrt{2}}\Big[\psi_1(x_1)\psi_1(x_3\downarrow)\psi_2(x_2\uparrow) - \psi_1(x_1)\psi_2(x_3\uparrow)\psi_1(x_2\downarrow)$$

$$+\psi_2(x_1)\psi_1(x_3\uparrow)\psi_1(x_2\downarrow) - \psi_2(x_1)\psi_1(x_3\downarrow)\psi_1(x_2\uparrow)\Big]$$

if we exchange particle 2 and 3 for the 2nd pure state:

in part ⑨: $\psi_1(x_1)\psi_2(x_2\uparrow)\psi_1(x_3\uparrow) \rightarrow \psi_1(x_1)\psi_2(x_3\uparrow)\psi_1(x_2\uparrow)$

in part ⑩: $-\psi_1(x_1)\psi_1(x_2\uparrow)\psi_2(x_3\uparrow) \rightarrow -\psi_1(x_1)\psi_1(x_3\uparrow)\psi_2(x_2\uparrow)$

hence: $\frac{1}{\sqrt{2}}\left[\psi_1(x_1)\psi_2(x_3\uparrow)\psi_1(x_2\uparrow) - \psi_1(x_1)\psi_1(x_3\uparrow)\psi_2(x_2\uparrow)\right]$

thus the remaining state is antisymmetric under exchange of particle 2 and 3.

Problem 3

This problem asks about the density matrix for two spin-1/2 particles in the singlet-triplet basis. Work with the quantization axis along $\hat{z}$.

(a) What is the density matrix if the system has 50% probability of being the $|\uparrow\downarrow\rangle_z$ state and 50% probability for being in the$|\uparrow\uparrow\rangle_x$ state?

(b) For the density matrix in (a), what is the probability that the system is in the singlet state? In the T_0 state?

(c) Introduce a zero-field spin splitting Δ for the triplet subsystem, which changes the relative energy of the T_0 compared wuth the T_+ and T_- states. Choose Δ such that the T_0 state has the lowest energy. What is the Hamiltonian for this term in matrix form?

Two spin ($-\frac{1}{2}$) have 4 eigenstates ($|\uparrow\uparrow\rangle$, $|\uparrow\downarrow\rangle$, $|\downarrow\uparrow\rangle$, $|\downarrow\downarrow\rangle$)

We use single-triplet basis to express $|\uparrow\downarrow\rangle_z$ and $|\uparrow\uparrow\rangle_x$

Triplets
$$\begin{cases} |T_+\rangle = |1,1\rangle = |\uparrow,\uparrow\rangle \\ |T_-\rangle = |1,-1\rangle = |\downarrow,\downarrow\rangle \\ |T_0\rangle = |1,0\rangle = \frac{1}{\sqrt{2}}(|\uparrow,\downarrow\rangle + |\downarrow,\uparrow\rangle) \end{cases}$$

Singlet $|S\rangle = |0,0\rangle = \frac{1}{\sqrt{2}}(|\uparrow,\downarrow\rangle - |\downarrow,\uparrow\rangle)$

So. $|\uparrow\downarrow\rangle_z = \dfrac{|T_0\rangle + |S\rangle}{\sqrt{2}}$

$$|\uparrow\uparrow\rangle_x = \frac{1}{2}(|\uparrow,\uparrow\rangle + |\uparrow,\downarrow\rangle + |\downarrow,\uparrow\rangle + |\downarrow,\downarrow\rangle)$$

$$= \frac{1}{2}|T_+\rangle + \frac{1}{2}|T_-\rangle + \frac{1}{\sqrt{2}}|T_0\rangle$$

pure state: $|\uparrow\downarrow\rangle_z\langle\uparrow\downarrow|_z$, $|\uparrow\uparrow\rangle_x\langle\uparrow\uparrow|_x$

So the density operator:

$$\rho = \sum_i W_i |\psi_i\rangle\langle\psi_i| = \frac{1}{2}|\uparrow\downarrow\rangle_z\langle\uparrow\downarrow|_z + \frac{1}{2}|\uparrow\uparrow\rangle_x\langle\uparrow\uparrow|_x$$

$$= \frac{1}{4}(|T_0\rangle + |S\rangle)(\langle T_0| + \langle S|) + \frac{1}{8}(|T_+\rangle + |T_-\rangle + \sqrt{2}|T_0\rangle)(\langle T_+| + \langle T_-| + \sqrt{2}\langle T_0|)$$

$$= \frac{1}{4}(|T_0\rangle\langle T_0| + |T_0\rangle\langle S| + |S\rangle\langle T_0| + |S\rangle\langle S|)$$

$$+\frac{1}{8}\Big(|T_+\rangle\langle T_+| + |T_+\rangle\langle T_-| + \sqrt{2}|T_+\rangle\langle T_0| + |T_-\rangle\langle T_+| + |T_-\rangle\langle T_-| + \sqrt{2}|T_-\rangle\langle T_0|$$

$$+\sqrt{2}|T_0\rangle\langle T_+| + \sqrt{2}|T_0\rangle\langle T_-| + 2|T_0\rangle\langle T_0|\Big)$$

$$= \frac{1}{4}\begin{pmatrix} 1 & 1 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} + \frac{1}{8}\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 2 & \sqrt{2} & \sqrt{2} \\ 0 & \sqrt{2} & 1 & 1 \\ 0 & \sqrt{2} & 1 & 1 \end{pmatrix} = \begin{pmatrix} \frac{1}{4} & \frac{1}{4} & 0 & 0 \\ \frac{1}{4} & \frac{1}{2} & \frac{\sqrt{2}}{8} & \frac{\sqrt{2}}{8} \\ 0 & \frac{\sqrt{2}}{8} & \frac{1}{8} & \frac{1}{8} \\ 0 & \frac{\sqrt{2}}{8} & \frac{1}{8} & \frac{1}{8} \end{pmatrix}$$

(b)

We use the projection measurement operators for singlet state and $|T_0\rangle$:

the probability in the singlet state:

$$P(|S\rangle) = Tr(\rho|S\rangle\langle S|) = \frac{1}{4}$$

the probability in the $|T_0\rangle$ state:

$$P(|T_0\rangle) = Tr(\rho|T_0\rangle\langle T_0|) = \frac{1}{2}$$

(c). consider a spin -1 system

$$\hat{S}_x = \frac{\hat{S}_+ + \hat{S}_-}{2} = \frac{\hbar}{\sqrt{2}}\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \quad \hat{S}_y = \frac{\hat{S}_+ - \hat{S}_-}{2i} = \frac{\hbar}{\sqrt{2}i}\begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 1 \\ 0 & -1 & 0 \end{pmatrix}$$

$$\hat{S}_z = \hbar\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

We express Hamiltonian as:

$$H = a\hat{S}_x^2 + b\hat{S}_y^2 + c\hat{S}_z^2$$

$$= a\frac{\hbar^2}{2}\begin{pmatrix} 1 & 0 & 1 \\ 0 & 2 & 0 \\ 1 & 0 & 1 \end{pmatrix} - b\frac{\hbar^2}{2}\begin{pmatrix} -1 & 0 & 1 \\ 0 & -2 & 0 \\ 1 & 0 & -1 \end{pmatrix} + c\hbar^2\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$$= \begin{pmatrix} \frac{a}{2}\hbar^2 + \frac{b}{2}\hbar^2 + c\hbar^2 & 0 & \frac{a}{2}\hbar^2 - \frac{b}{2}\hbar^2 \\ 0 & a\hbar^2 + b\hbar^2 & 0 \\ \frac{a}{2}\hbar^2 - \frac{b}{2}\hbar^2 & 0 & \frac{a}{2}\hbar^2 + \frac{b}{2}\hbar^2 + c\hbar^2 \end{pmatrix}$$

here. we may assume $a = b$. and c is free.

So $H = \begin{pmatrix} a\hbar^2 + c\hbar^2 & 0 & 0 \\ 0 & 2a\hbar^2 & 0 \\ 0 & 0 & a\hbar^2 + c\hbar^2 \end{pmatrix}$

We have the equation: $(H - EI)|\psi\rangle = 0$. I is the identity matrix.

$$\det \begin{vmatrix} a\hbar^2 + c\hbar^2 - E & 0 & 0 \\ 0 & 2a\hbar^2 - E & 0 \\ 0 & 0 & a\hbar^2 + c\hbar^2 - E \end{vmatrix} = 0 \Rightarrow \begin{cases} E_1 = (a+c)\hbar^2 & (T_+ \text{ state}) \\ E_2 = 2a\hbar^2 & (T_0 \text{ state}) \\ E_3 = (a+c)\hbar^2 & (T_- \text{ state}) \end{cases}$$

Considering the zero field splitting that changes the relative energy of T_0 compared with T_+, T_- state.

So the difference of T_+ and T_0 states (T_- and T_0 states) is denoted as: $E_1 - E_2 = E_3 - E_2 = (c-a)\hbar^2 = \Delta$

because $a + b + c = 0$, $\begin{cases} 2a + c = 0 \\ (c-a)\hbar^2 = \Delta \end{cases} \Rightarrow \begin{cases} a = \dfrac{\Delta}{-3\hbar^2} \\ c = \dfrac{2\Delta}{3\hbar^2} \end{cases}$

H matrix: $H = \hbar^2 \begin{pmatrix} \frac{\Delta}{3\hbar^2} & 0 & 0 \\ 0 & -\frac{2}{3\hbar^2}\Delta & 0 \\ 0 & 0 & \frac{\Delta}{3\hbar^2} \end{pmatrix}$