Problem Set #3

Problem 1

Since $\rho_{mixed} = \sum_i p_i |\psi_i\rangle\langle\psi_i|$

$$\begin{aligned}\hat{\rho} = \frac{1}{5}| \uparrow_Y\rangle\langle\uparrow_Y | + \frac{4}{5}| \downarrow_Y\rangle\langle\downarrow_Y | &= \frac{1}{5}\left(\frac{1}{2}\right)\begin{pmatrix}1\\ i\end{pmatrix}\begin{pmatrix}1 & -i\end{pmatrix} + \frac{4}{5}\left(\frac{1}{2}\right)\begin{pmatrix}1\\ -i\end{pmatrix}\begin{pmatrix}1 & i\end{pmatrix} \\ &= \frac{1}{10}\begin{pmatrix}1 & -i\\ i & 1\end{pmatrix} + \frac{4}{10}\begin{pmatrix}1 & i\\ -i & 1\end{pmatrix} = \begin{pmatrix}\frac{1}{2} & \frac{3}{10}i\\ \frac{-3}{10}i & \frac{1}{2}\end{pmatrix}\end{aligned} \tag{1.1}$$

2 points given for correctly identifying that this is a mixed state.
1 point given for using the correct spin basis states.
1 point given for the correct density matrix.
Evaluating the expectation values:

$$Tr[\hat{\rho}\hat{S}_z] = \frac{\hbar}{2}Tr[\hat{\rho}\sigma_z] = Tr\left[\frac{\hbar}{2}\begin{pmatrix}\frac{1}{2} & \frac{3}{10}i\\ \frac{-3}{10}i & \frac{1}{2}\end{pmatrix}\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}\right] = \frac{\hbar}{2}Tr\left[\begin{pmatrix}\frac{1}{2} & -\frac{3}{10}i\\ \frac{-3}{10}i & -\frac{1}{2}\end{pmatrix}\right] = 0 \tag{1.2}$$

$$Tr[\hat{\rho}\hat{S}_x] = \frac{\hbar}{2}Tr[\hat{\rho}\sigma_x] = Tr\left[\frac{\hbar}{2}\begin{pmatrix}\frac{1}{2} & \frac{3}{10}i\\ \frac{-3}{10}i & \frac{1}{2}\end{pmatrix}\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}\right] = Tr\left[\frac{\hbar}{2}\begin{pmatrix}\frac{3}{10}i & \frac{1}{2}\\ \frac{1}{2} & -\frac{7}{10}i\end{pmatrix}\right] = 0 \tag{1.3}$$

1 point given for each correct expectation value (2 points total).
1 point for writing the expectation value as the trace of ρ times the operator. (2 points total).

Problem 2

The wavefunction from HW#2 2(b) is:

$$|\Psi\rangle = 6^{-1/2}\left(f_{123}\left|\uparrow\downarrow\uparrow\right\rangle - f_{132}\left|\uparrow\uparrow\downarrow\right\rangle - f_{213}\left|\downarrow\uparrow\uparrow\right\rangle + f_{312}\left|\downarrow\uparrow\uparrow\right\rangle + f_{231}\left|\uparrow\uparrow\downarrow\right\rangle - f_{321}\left|\uparrow\downarrow\uparrow\right\rangle\right) \tag{2.1}$$

where $f_{\alpha\beta\gamma} = \psi_1(x_\alpha)\,\psi_1(x_\beta)\,\psi_2(x_\gamma)$
1 point for using the correct wavefunction from homework 2. ρ is calculated via:

$$\hat{\rho} = |\Psi\rangle\langle\Psi| \tag{2.2}$$

1 point for identifying the density matrix as the outer product of the wavefunction. Taking the trace of the density matrix over spinor 1 is

$$\mathrm{tr}_{s1}[\rho] = 6^{-1}\begin{pmatrix}(f_{312}-f_{213})(f_{312}-f_{213})^\dagger & 0 & 0 & 0\\ 0 & (f_{231}-f_{132})(f_{231}-f_{132})^\dagger & (f_{231}-f_{132})(f_{123}-f_{321})^\dagger & 0\\ 0 & (f_{123}-f_{321})(f_{231}-f_{132})^\dagger & (f_{123}-f_{321})(f_{123}-f_{321})^\dagger & 0\\ 0 & 0 & 0 & 0\end{pmatrix} \tag{2.3}$$

1 point for the correct density matrix.
1 point for identifying the form of the partial trace.
1 point for correct density matrix after taking the partial trace over particle 1's spin. Note that this result must be properly normalized.
1 point for finding the wavefunction from each pure state density matrix (2 points total). Note that these wavefunctions must be properly normalized.
We now exchange particle 2&3 only in the kets. Note that both the spacial and spinor has to be swapped, i.e. swapping 2&3 in the index of f, and the 2nd&3rd row of the matrix.

$$\begin{aligned}
&\mathrm{SWAP}_{23}\mathrm{tr}_{s1}\left[\rho\right] \\
=&6^{-1}\begin{pmatrix}
(f_{213}-f_{312})(f_{312}-f_{213})^\dagger & 0 & 0 & 0 \\
0 & (f_{132}-f_{231})(f_{231}-f_{132})^\dagger & (f_{132}-f_{231})(f_{123}-f_{321})^\dagger & 0 \\
0 & (f_{321}-f_{123})(f_{231}-f_{132})^\dagger & (f_{321}-f_{123})(f_{123}-f_{321})^\dagger & 0 \\
0 & 0 & 0 & 0
\end{pmatrix} \\
=&6^{-1}\begin{pmatrix}
-(f_{312}-f_{213})(f_{312}-f_{213})^\dagger & 0 & 0 & 0 \\
0 & -(f_{231}-f_{132})(f_{231}-f_{132})^\dagger & -(f_{231}-f_{132})(f_{123}-f_{321})^\dagger & 0 \\
0 & -(f_{123}-f_{321})(f_{231}-f_{132})^\dagger & -(f_{123}-f_{321})(f_{123}-f_{321})^\dagger & 0 \\
0 & 0 & 0 & 0
\end{pmatrix} \\
=&-\mathrm{tr}_{s1}\left[\rho\right]
\end{aligned} \tag{2.4}$$

1 point for work that shows exchange of the particles in each wave function. (2 points total). This must be shown explicitly.
1 point for showing the antisymmetry requirement for each wavefunction in the density matrix (2 points total).

Problem 3

(a) For this problem it is convenient to work in the single/triplet basis ($|S\rangle$,$|T_0\rangle$,$|T_+\rangle$,$|T_-\rangle$). The $|\uparrow\downarrow\rangle_z$ state can be expressed as:

$$|\uparrow\downarrow\rangle_z = \frac{|S\rangle + |T_0\rangle}{\sqrt{2}} \tag{3.1}$$

And the $|\uparrow\uparrow\rangle$ state can be written as:

$$|\uparrow\uparrow\rangle_x = \frac{1}{2}(|\uparrow\uparrow\rangle_z + |\uparrow\downarrow\rangle_z + |\downarrow\uparrow\rangle_z + |\downarrow\downarrow\rangle_z) = \frac{1}{2}(|T_+\rangle + |T_-\rangle + \sqrt{2}|T_0\rangle) \tag{3.2}$$

1 point for correctly writing each state in the singlet triplet basis. (2 points total). The state can alternatively be written in the spin product basis.

The density matrix is then:

$$
\begin{aligned}
\hat{\rho} &= \frac{1}{2}|\uparrow\downarrow\rangle_z\langle\uparrow\downarrow|_z + \frac{1}{2}|\uparrow\uparrow\rangle_x\langle\uparrow\uparrow|_x \\
&= \frac{1}{4}\left(|S\rangle + |T_0\rangle\right)\left(\langle S| + \langle T_0|\right) + \frac{1}{8}\left(|T_+\rangle + |T_-\rangle + \sqrt{2}|T_0\rangle\right)\left(\langle T_+| + \langle T_-| + \sqrt{2}\langle T_0|\right) \\
&= \begin{pmatrix} \frac{1}{4} & \frac{1}{4} & 0 & 0 \\ \frac{1}{4} & \frac{1}{4} & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & \frac{1}{4} & \frac{\sqrt{2}}{8} & \frac{\sqrt{2}}{8} \\ 0 & \frac{\sqrt{2}}{8} & \frac{1}{8} & \frac{1}{8} \\ 0 & \frac{\sqrt{2}}{8} & \frac{1}{8} & \frac{1}{8} \end{pmatrix} \\
&= \begin{pmatrix} \frac{1}{4} & \frac{1}{4} & 0 & 0 \\ \frac{1}{4} & \frac{1}{2} & \frac{\sqrt{2}}{8} & \frac{\sqrt{2}}{8} \\ 0 & \frac{\sqrt{2}}{8} & \frac{1}{8} & \frac{1}{8} \\ 0 & \frac{\sqrt{2}}{8} & \frac{1}{8} & \frac{1}{8} \end{pmatrix}
\end{aligned}
\tag{3.3}
$$

Note that for this result $Tr[\hat{\rho}] = 1$.
1 point for identifying the density matrix as that of a mixed state.
1 point for the correct density matrix.

(b) Note that we can read off P_{singlet} in this basis.

$$P_{\text{singlet}} = \langle S|\hat{\rho}|S\rangle = \frac{1}{4} \tag{3.4}$$

Likewise:

$$P_{\text{T0}} = \langle T_0|\hat{\rho}|T_0\rangle = \frac{1}{2} \tag{3.5}$$

1 point for each correct probability calculated. (2 points total)

(c) One way to express the Hamiltonian in this basis is:

$$\hat{H} = -\Delta|T_0\rangle\langle T_0| = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & -\Delta & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \tag{3.6}$$

For $\Delta > 0$.
3 points if the correct energy difference is obtained between the T_0 state and the other 2 triplet states. (1 point if a matrix is written but incorrect, or gives a splitting of 2Δ).