Problem Set #2

Problem 1

The Hamiltonian is:

$$\hat{H} = \frac{\hat{P}^2}{2m} \tag{1.1}$$

The translation operator is denoted $\hat{T}_a$, such that:

$$\hat{T}_a f(x) = f(x+a) \tag{1.2}$$

for all f(x). The inversion operator is denoted $\hat{I}$, such that:

$$\hat{I} f(x) = f(-x) \tag{1.3}$$

and

$$\hat{P}\hat{I} f(x) = -\hat{P} f(-x) \tag{1.4}$$

for all $f(x)$.

(a) The commutator $\big[\hat{H}, \hat{T}_a\big]$ is:

$$\big[\hat{H}, \hat{T}_a\big] f(x) = \hat{H}\hat{T}_a f(x) - \hat{T}_a \hat{H} f(x) = \hat{H} f(x+a) - \hat{T}_a \hat{H} f(x) \tag{1.5}$$

Since,

$$\hat{H} f(x) = \frac{-\hbar^2 d^2}{2m dx^2} f(x) = -\frac{\hbar^2}{2m} f''(x) \tag{1.6}$$

So,

$$\begin{aligned} \big[\hat{H}, \hat{T}_a\big] f(x) &= \frac{-\hbar^2}{2m} f''(x+a) - \hat{T}_a \left(\frac{-\hbar^2}{2m} f''(x) \right) \\ &= \frac{-\hbar^2}{2m} \big[f''(x+a) - \hat{T}_a f''(x) \big] = \frac{-\hbar^2}{2m} \big[f''(x+a) - f''(x+a) \big] = 0 \end{aligned} \tag{1.7}$$

2 points for showing the commutator of $\hat{T}_a$, and $\hat{H}$ by explicit form of the Hamiltonian. Note, it is not enough here to state that the Hamiltonian has translational symmetry without explicit argument. If the commutator was evaluated this way, 1 point was given.
The commutator $\big[\hat{H}, \hat{I}\big]$ may be calculated similarly:

$$\big[\hat{H}, \hat{I}\big] = \frac{-\hbar^2}{2m} \left[\frac{d^2 f^*(-x)}{dx^2} - \hat{I} f''(x) \right] \tag{1.8}$$

Since,

$$\frac{d^2}{dx^2} f(-x) = \frac{d}{dx}\big(- f'(-x) \big) = f''(-x) \tag{1.9}$$

$$\left[\hat{H}, \hat{I}\right] = \frac{-\hbar^2}{2m}\left[f''(-x) - \hat{I}f''(x)\right] = 0 \tag{1.10}$$

2 points for showing the commutator of $\hat{H}$, and $\hat{I}$ by explicit form of the Hamiltonian. Note, it is not enough to state here that the Hamiltonian has inversion symmetry without explicit argument. If the commutator was evaluated this way, 1 point was given.

(b) The commutator:

$$\left[\hat{T}_a, \hat{I}\right]f(x) = \left(\hat{T}_a\hat{I} - \hat{I}\hat{T}_a\right)f(x) = f(-x+a) - f(-x-a) \neq 0 \tag{1.11}$$

for generic $f(x)$.
2 points for evaluating the commutator correctly.

(c) The inversion operator may be directly evaluated on the state $\psi_p(x)$:

$$\hat{I}\psi_p(x) = \hat{I}V^{-1/2}e^{ipx/\hbar} = V^{-1/2}e^{ip(-x)/\hbar} = V^{-1/2}e^{-ipx/\hbar} = V^{-1/2}e^{i(-p)x/\hbar} = \psi_{-p}(x) \tag{1.12}$$

2 point for showing correct behavior of the inversion operator.
Furthermore, these states have the same energy since $\hat{H}$ and $\hat{I}$ commute.

$$\hat{H}\hat{I}\psi_p(x) = \hat{I}\hat{H}\psi_p(x) \tag{1.13}$$

So,

$$\hat{H}\psi_{-p} = \hat{I}E_p\psi_p(x) \tag{1.14}$$

and therefore:

$$E_{-p}\psi_{-p}(x) = E_p\hat{I}\psi_p(x) = E_p\psi_{-p}(x) \tag{1.15}$$

Here we can see that $E_{-p} = E_p$.

(d) We just need to evaluate the translation operator on one of these states to show that they are mixed.

$$\begin{aligned}
\hat{T}_a(\pi\hbar)^{-1/2}\cos(px/\hbar) &= (\pi\hbar)^{-1/2}\cos(p(x+a)/\hbar) = (\pi\hbar)^{-1/2}\cos\left(\frac{px}{\hbar} + \frac{pa}{\hbar}\right) \\
&= (\pi\hbar)^{-1/2}\left(\cos\left(\frac{px}{\hbar}\right)\cos\left(\frac{pa}{\hbar}\right) - \sin\left(\frac{px}{\hbar}\right)\sin\left(\frac{pa}{\hbar}\right)\right) \\
&= \cos\left(\frac{pa}{\hbar}\right)\left[(\pi\hbar)^{-1/2}\cos\left(\frac{px}{\hbar}\right)\right] - \sin\left(\frac{pa}{\hbar}\right)\left[(\pi\hbar)^{-1/2}\sin\left(\frac{px}{\hbar}\right)\right]
\end{aligned} \tag{1.16}$$

Clearly the states are mixed and since $\left[\hat{T}_a, \hat{H}\right] = 0$ they are also degenerate.
1 point for correct evaluation of the translation operator.

Problem 2

(a) First, the fully symmetric wavefunction constructed from 3 spins:

$$\psi = a_1|\uparrow\uparrow\uparrow\rangle + a_2|\uparrow\uparrow\downarrow\rangle + a_3|\uparrow\downarrow\uparrow\rangle + a_4|\uparrow\downarrow\downarrow\rangle + a_5|\downarrow\uparrow\uparrow\rangle + a_6|\downarrow\uparrow\downarrow\rangle + a_7|\downarrow\downarrow\uparrow\rangle + a_8|\downarrow\downarrow\downarrow\rangle \tag{2.1}$$

1 point for constructing the correct wavefunction
Requiring antisymmetry of exchange of particle 1 and particle 2 gives:

$$\psi(2,1,3) = -\psi(1,2,3) \tag{2.2}$$

Now calculate the wavefunction under exchange:

$$\psi(2,1,3) = a_1|\uparrow\uparrow\uparrow\rangle + a_2|\uparrow\uparrow\downarrow\rangle + a_5|\uparrow\downarrow\uparrow\rangle + a_6|\uparrow\downarrow\downarrow\rangle + a_3|\downarrow\uparrow\uparrow\rangle + a_4|\downarrow\uparrow\downarrow\rangle + a_7|\downarrow\downarrow\uparrow\rangle + a_8|\downarrow\downarrow\downarrow\rangle \tag{2.3}$$

The antisymmetry requirement constrains $a_1 = -a_1$, $a_2 = -a_2$,$a_7 = -a_7$, $a_8 = -a_8$, $a_5 = -a_3$, and $a_4 = -a_6$. This means that a_1,a_2,a_7, and a_8 are all equal to 0.
1 point for correct calculation of the coefficients under 1-2 exchange. Points were not given if constraints on any of the coefficients were left out.
The wavefunction is now:

$$\psi(1,2,3) = a_3|\uparrow\downarrow\uparrow\rangle - a_3|\downarrow\uparrow\uparrow\rangle + a_4|\uparrow\downarrow\downarrow\rangle - a_4|\downarrow\uparrow\downarrow\rangle \tag{2.4}$$

Because we also require that the wavefunction is symmetric under exchange of particles 2 and 3, $-\psi(1,2,3) = \psi(1,3,2)$:
1 point for correct calculation of the coefficients under 2-3 exchange. Points were not given if any constraints on the remaining coefficients were left out.

$$\psi(1,3,2) = a_3|\uparrow\uparrow\downarrow\rangle - a_3|\downarrow\uparrow\uparrow\rangle + a_4|\uparrow\downarrow\downarrow\rangle - a_4|\downarrow\downarrow\uparrow\rangle \tag{2.5}$$

Since $-a_3 = a_3$ and $-a_4 = a_4$ as required by antisymmetry, all coefficients must equal 0. Therefore there is no antisymmetric wavefunction possible.
Alternatively, the 8-dimensional space is spanned by the 8 "computational" states, which are eigenvectors of at least 1 exchange operator with eigenvalue 1, namely

$$\begin{aligned}
\mathrm{SWAP}_{12}\left(a_1|\uparrow\uparrow\uparrow\rangle + a_2|\uparrow\uparrow\downarrow\rangle + a_7|\downarrow\downarrow\uparrow\rangle + a_8|\downarrow\downarrow\downarrow\rangle\right) &= a_1|\uparrow\uparrow\uparrow\rangle + a_2|\uparrow\uparrow\downarrow\rangle + a_7|\downarrow\downarrow\uparrow\rangle + a_8|\downarrow\downarrow\downarrow\rangle \\
\mathrm{SWAP}_{13}\left(a_1|\uparrow\uparrow\uparrow\rangle + a_3|\uparrow\downarrow\uparrow\rangle + a_6|\downarrow\uparrow\downarrow\rangle + a_8|\downarrow\downarrow\downarrow\rangle\right) &= a_1|\uparrow\uparrow\uparrow\rangle + a_3|\uparrow\downarrow\uparrow\rangle + a_6|\downarrow\uparrow\downarrow\rangle + a_8|\downarrow\downarrow\downarrow\rangle \\
\mathrm{SWAP}_{23}\left(a_1|\uparrow\uparrow\uparrow\rangle + a_4|\uparrow\downarrow\downarrow\rangle + a_5|\downarrow\uparrow\uparrow\rangle + a_8|\downarrow\downarrow\downarrow\rangle\right) &= a_1|\uparrow\uparrow\uparrow\rangle + a_4|\uparrow\downarrow\uparrow\rangle + a_5|\downarrow\uparrow\uparrow\rangle + a_8|\downarrow\downarrow\downarrow\rangle
\end{aligned} \tag{2.6}$$

Since SWAP operator is Hermitian, eigenvectors with different eigenvalues must be orthogonal, so If there exists a completely antisymmetric state, i.e. eigenstate of all 3 SWAP operators with eigenvalue -1, it must be orthogonal to all 8 basis states, in other words outside of this space.

(b) We denote the wavefunctions of the infinite square well as:

$$\psi_n(x) = \left(\frac{2}{a}\right)^{1/2} \sin\left(\frac{n\pi x}{a}\right) \tag{2.7}$$

$\psi_n(x)$ are the spatial part of the wavefunction, and χ_+, and χ_- denote the spin part of the wavefunction.

Method 1: Direct approach (motivated from (c))

For three spin 1/2 fermions in a square infinite potential well, the total ground state should be two particle fill up the ground state and one particle fill up the first excited state. Sot the total energy is

$$E = 2E_1 + E_2 = \frac{3\pi^2\hbar^2}{ma^2} \tag{2.8}$$

Let's construct the complete anti-symmetric state:
First, with 2 fermion at lowest ground state $\psi_1(x)$, we have

$$\psi(i,j) = \psi_1(x_i)\psi_2(x_j)(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)/\sqrt{2} \tag{2.9}$$

Then we add the third Fermion on the first excited state $\psi_2(x)$ and construct a generic three particle state

$$\psi(1,2,3) = \psi(1,2)\psi_2(x_3)(c_1|\uparrow\rangle + c_2|\downarrow\rangle) + \psi(2,3)\psi_2(x_1)(c_3|\uparrow\rangle + c_4|\downarrow\rangle) + \psi(3,1)\psi_2(x_2)(c_5|\uparrow\rangle + c_6|\downarrow\rangle) \tag{2.10}$$

Then we require complete antisymmetry of $\psi(1,2,3)$ which gives $c_1 = c_3 = c_5$ and $c_2 = c_4 = c_6$. So we get two orthogonal degenerate states

$$\begin{aligned}\psi(1,2,3)_{\uparrow_2} = \frac{1}{\sqrt{3!}}\big[&\psi_{2,\uparrow}(x_1)\left(\psi_{1,\uparrow}(x_2)\psi_{1,\downarrow}(x_3) - \psi_{1,\downarrow}(x_2)\psi_{1,\uparrow}(x_3)\right)\\ &- \psi_{2,\uparrow}(x_2)\left(\psi_{1,\uparrow}(x_1)\psi_{1,\downarrow}(x_3) - \psi_{1,\downarrow}(x_3)\psi_{1,\uparrow}(x_1)\right)\\ &+ \psi_{2,\uparrow}(x_3)\left(\psi_{1,\uparrow}(x_1)\psi_{1,\downarrow}(x_2) - \psi_{1,\downarrow}(x_2)\psi_{1,\uparrow}(x_1)\right)\big]\end{aligned} \tag{2.11}$$

$$\begin{aligned}\psi(1,2,3)_{\downarrow_2} = \frac{1}{\sqrt{6}}\big[&\psi_{2,\downarrow}(x_1)\left(\psi_{1,\uparrow}(x_2)\psi_{1,\downarrow}(x_3) - \psi_{1,\downarrow}(x_2)\psi_{1,\uparrow}(x_3)\right)\\ &- \psi_{2,\downarrow}(x_2)\left(\psi_{1,\uparrow}(x_1)\psi_{1,\downarrow}(x_3) - \psi_{1,\downarrow}(x_3)\psi_{1,\uparrow}(x_1)\right)\\ &+ \psi_{2,\downarrow}(x_3)\left(\psi_{1,\uparrow}(x_1)\psi_{1,\downarrow}(x_2) - \psi_{1,\downarrow}(x_2)\psi_{1,\uparrow}(x_1)\right)\big]\end{aligned} \tag{2.12}$$

$\uparrow_2$ and $\downarrow_2$ denotes the particle on first excited state $\psi_2(x)$ has the spin up or spin down.

Method 2: Slater determinant

The antisymmetrized wavefunction is given by the Slater determinant:

$$\psi(1,2,3) = \frac{1}{\sqrt{8}}\det\begin{bmatrix}\psi_1(x_1)\chi_+(1) & \psi_1(x_1)\chi_-(1) & \psi_2(x_1)\chi_+(1)\\ \psi_1(x_2)\chi_+(2) & \psi_1(x_2)\chi_-(2) & \psi_2(x_2)\chi_+(2)\\ \psi_1(x_3)\chi_+(3) & \psi_1(x_3)\chi_-(3) & \psi_2(x_3)\chi_+(3)\end{bmatrix} \tag{2.13}$$

2 points for constructing the Slater determinant. Partial credit is given if approach is correct but final wavefunction is wrong/unnormalized. The spin for the particle in

the excited state does not need to be specified if the degeneracy was also correctly identified.
This equals:

$$\begin{aligned}\frac{1}{\sqrt{6}}[&\psi_1(x_1)\psi_1(x_2)\psi_2(x_3)\chi_+(1)\chi_-(2)\chi_+(3) - \psi_1(x_1)\psi_2(x_2)\psi_1(x_3)\chi_+(1)\chi_+(2)\chi_-(3)\\ &-\psi_1(x_1)\psi_1(x_2)\psi_2(x_3)\chi_-(1)\chi_+(2)\chi_+(3) + \psi_1(x_1)\psi_2(x_2)\psi_1(x_3)\chi_-(1)\chi_+(2)\chi_+(3)\\ &+\psi_2(x_1)\psi_1(x_2)\psi_1(x_3)\chi_+(1)\chi_+(2)\chi_-(3) - \psi_2(x_1)\psi_1(x_2)\psi_1(x_3)\chi_+(1)\chi_-(2)\chi_+(3)]\end{aligned} \tag{2.14}$$

The energy of this state is given by:

$$2E_1 + E_2 = 2\left(\frac{\pi^2\hbar^2}{2ma^2}\right) + \left(\frac{2^2\pi^2\hbar^2}{2ma^2}\right) = 6E_1 = \left(\frac{3\pi^2\hbar^2}{ma^2}\right) \tag{2.15}$$

2 points for correct calculation of the energy. Partial credit given for approach is correct but units are wrong.
Since the 3rd state in the slater determinant could be spin up or down the degeneracy is 2.
1 point for correct calculation of the degeneracy.

(c) Denoting $\Phi(i,j) = \psi_1(i)\chi_+(i)\psi_1(j)\chi_-(j) - \psi_1(i)\chi_-(i)\psi_1(j)\chi_+(j)$, and $\phi(k) = \psi_2(k)\chi_+(k)$. Then

$$\psi(1,2,3) = \frac{1}{\sqrt{3}}[\Phi(1,2)\phi(3) - \Phi(1,3)\phi(2) + \Phi(2,3)\phi(1)] \tag{2.16}$$

1 point for correctly rewriting the wavefunction in the given form. Had to correctly identify the form of $\Phi(i,j)$, and $\phi(k)$ and show how the normalization changes. Points were not given if the $\phi(k)$ spin remained unspecified from part 2(b).
Now to check that $\psi(1,2,3)$ is antisymmetric under all three exchanges of 2 particles, note that:

$$\Phi(i,j) = -\Phi(j,i) \tag{2.17}$$

The proof:

$$\begin{aligned}\Phi(i,j) &= \psi_1(i)\chi_+(i)\psi_1(j)\chi_-(j) - \psi_1(i)\chi_-(i)\psi_1(j)\chi_+(j)\\ &= -\left(\psi_1(j)\chi_+(j)\psi_1(i)\chi_-(i) - \psi_1(j)\chi_-(j)\psi_1(i)\chi_+(i)\right)\\ &= -\Phi(j,i)\end{aligned} \tag{2.18}$$

1 point for identifying the antisymmetry of $\Phi(i,j)$.
Now exchanging particles 1 and 2 in the total wavefunction:

$$\begin{aligned}\psi(1,2,3) \to \Phi(2,1,3) &= \frac{1}{\sqrt{3}}\big[\Phi(2,1)\phi(3) - \Phi(2,3)\phi(1) + \Phi(1,3)\phi(2)\big]\\ &= \frac{1}{\sqrt{3}}\big[-\Phi(1,2)\phi(3) + \Phi(1,3)\phi(2) - \Phi(2,3)\phi(1)\big]\\ &= \frac{-1}{\sqrt{3}}\big[\Phi(1,2)\phi(3) - \Phi(1,3)\phi(2) + \Phi(2,3)\phi(1)\big] = -\psi(1,2,3)\end{aligned} \tag{2.19}$$

1 point for showing exchange of 1 and 2. Needed to show how individual terms in the wavefunction pick up a sign under exchange.
Exchanging particles 2 and 3 in the total wavefunction:

$$\begin{aligned}\psi(1,3,2) &= \frac{1}{\sqrt{3}}\big[\Phi(1,3)\phi(2) - \Phi(1,2)\phi(3) + \Phi(3,2)\phi(1)\big] \\ &= \frac{1}{\sqrt{3}}\big[\Phi(1,3)\phi(2) - \Phi(1,2)\phi(3) - \Phi(2,3)\phi(1)\big] \\ &= \frac{-1}{\sqrt{3}}\big[\Phi(1,2)\phi(3) - \Phi(1,3)\phi(2) + \Phi(2,3)\phi(1)\big] = -\psi(1,2,3)\end{aligned} \tag{2.20}$$

1 point for showing exchange of 2 and 3. Needed to show how individual terms in the wavefunction pick up a sign under exchange.
Exchanging particles 1 and 3:

$$\begin{aligned}\psi(3,2,1) &= \frac{1}{\sqrt{3}}\big[\Phi(3,2)\phi(1) - \Phi(3,1)\phi(2) + \Phi(2,1)\phi(3)\big] \\ &= \frac{1}{\sqrt{3}}\big[\Phi(2,3)\phi(1) + \Phi(1,3)\phi(2) - \Phi(1,2)\phi(3)\big] \\ &= \frac{-1}{\sqrt{3}}\big[\Phi(1,2)\phi(3) - \Phi(1,3)\phi(2) + \Phi(2,3)\phi(1)\big] = -\psi(1,2,3)\end{aligned} \tag{2.21}$$

1 point for showing exchange of 1 and 3. Requires showing how individual terms in the wavefunction pick up a sign under exchange.

Problem 3

(a) Similar to HW1 problem 2.

$$H = \begin{bmatrix} \epsilon/2 & \Delta/2 \\ \Delta/2 & -\epsilon/2 \end{bmatrix} \tag{3.1}$$

The eigenenergies are

$$E_\pm = \pm\frac{1}{2}\sqrt{\epsilon^2 + \Delta^2} \tag{3.2}$$

Eigenvectors are

$$|\psi_\pm\rangle = \frac{1}{(-\epsilon/\lambda \pm \sqrt{\epsilon^2/\lambda^2 + 1})^2 + 1)]}[(-\epsilon/\lambda \pm \sqrt{\epsilon^2/\lambda^2 + 1})|L\rangle + |R\rangle] \tag{3.3}$$

The transition frequency

$$\omega_0 = \frac{1}{\hbar}\sqrt{\epsilon^2 + \Delta^2} \tag{3.4}$$

1 point each for eigenenergies, eigenstates, and frequency

(b) Using the relation between Δ and λ, we know

$$d\lambda = -d\Delta/\Delta \tag{3.5}$$

Using the relation $E = \sqrt{\epsilon^2 + \Delta^2}$, we substitute $d\epsilon = \frac{EdE}{\sqrt{E^2-\Delta^2}}$ and integrate over Δ

$$\int D(E)dE = \int\int P_0 d\epsilon \frac{d\Delta}{\Delta} = P_0 \int dE \int_{\Delta_0}^{E} d\Delta \frac{E}{\Delta\sqrt{E^2-\Delta^2}} \tag{3.6}$$

$$D(E) = P_0 \int_{\Delta_0}^{E} \frac{E}{\Delta\sqrt{E^2-\Delta^2}}\, d\Delta = P_0 \operatorname{arctanh}\sqrt{1-\Delta_0^2/E^2} = P_0 \ln\frac{E+\sqrt{E^2-\Delta_0^2}}{\Delta_0} \tag{3.7}$$

1 point each for double integral for total number of states, density as derivative of total number of states, and correct final expression

(c) According to FGR and resonant coupling condition

$$R_{tot} = \frac{2\pi}{\hbar^2}\int D(E)|J_{TLS}|^2\delta(\frac{E}{\hbar}-\omega_0)dE = \frac{2\pi}{\hbar}P_0|J_{TLS}|^2 \operatorname{arctanh}\sqrt{1-\Delta_0^2/(\hbar\omega_0)^2} \tag{3.8}$$

$$= \frac{2\pi}{\hbar}P_0|J_{TLS}|^2 \ln\frac{(\hbar\omega_0)+\sqrt{(\hbar\omega_0)^2-\Delta_0^2}}{\Delta_0} \tag{3.9}$$

1 point each for correct equation and final expression