Advanced Quantum Mechanics: Fall 2017
Final Exam: Brief Solutions

NOTE: Sentences in italic fonts are questions to be answered.

Possibly Useful facts:

- $\epsilon^{abc} \equiv \begin{cases} +1, & abc = xyz, \text{ or } yzx, \text{ or } zxy; \\ -1, & abc = zyx, \text{ or } xzy, \text{ or } yxz; \\ 0, & \text{otherwise.} \end{cases}$ $\epsilon^{abc} = \epsilon^{bca} = \epsilon^{cab} = \epsilon^{-acb} = \epsilon^{-bac} = \epsilon^{-cba}$.

  $\delta_{ab} \equiv \begin{cases} 1, & a = b; \\ 0, & a \neq b. \end{cases}$ $\sum_c \epsilon^{abc}\epsilon^{cdf} = \delta_{ad}\delta_{bf} - \delta_{af}\delta_{bd}$.

- Some Taylor expansions: $\exp(x) = \sum_{n=0}^{\infty} \frac{x^n}{n!} = 1 + x + \frac{x^2}{2} + \frac{x^3}{6} + O(x^4)$,

  $\sqrt{1+x} = 1 + \frac{1}{2}x - \frac{1}{8}x^2 + O(x^3)$, $\frac{1}{\sqrt{1+x}} = 1 - \frac{1}{2}x + \frac{3}{8}x^2 + O(x^3)$.

- Baker-Hausdorff formula: $\exp(\hat{A}) \cdot \hat{B} \cdot \exp(-\hat{A}) = \hat{B} + \sum_{n=1}^{+\infty} \frac{1}{n!} \underbrace{[\hat{A}, [\hat{A}, \ldots [\hat{A},}_{n\text{-fold commutator}} \hat{B}] \ldots]]$.

- Spin (angular momentum) operators satisfy $[\hat{S}_a, \hat{S}_b] = \mathbb{i} \sum_c \epsilon^{abc} \hat{S}_c$.

  Ladder operators $\hat{S}_\pm \equiv \hat{S}_x \pm \mathbb{i}\hat{S}_y$, and $[\hat{S}_z, \hat{S}_\pm] = \pm\hat{S}_\pm$, and

  $\hat{S}_\pm |S, S_z = m\rangle = \sqrt{(S \mp m)(S \pm m + 1)} |S, S_z = m \pm 1\rangle$.

- $\hat{\boldsymbol{S}}_i \cdot \hat{\boldsymbol{S}}_j \equiv \hat{S}_{iz}\hat{S}_{jz} + \hat{S}_{ix}\hat{S}_{jx} + \hat{S}_{iy}\hat{S}_{jy} = \hat{S}_{iz}\hat{S}_{jz} + \frac{1}{2}(\hat{S}_{i+}\hat{S}_{j-} + \hat{S}_{i-}\hat{S}_{j+})$.

- Spin-1/2: $\hat{S}_a = \sigma_a/2$ under the $\hat{S}_z$ eigenbasis, for $a = x, y, z$.

  The Pauli matrices σ_a are $\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$, $\sigma_y = \begin{pmatrix} 0 & -\mathbb{i} \\ \mathbb{i} & 0 \end{pmatrix}$, $\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$. $\{\sigma_a, \sigma_b\} = 2\delta_{ab}\mathbb{1}$.

  $\exp(-\mathbb{i}\theta \boldsymbol{n} \cdot \boldsymbol{\sigma}) = \cos(\theta)\mathbb{1} - \mathbb{i}\sin(\theta)(\boldsymbol{n} \cdot \boldsymbol{\sigma})$, for unit-length 3-component real vector $\boldsymbol{n}$.

  (here $\boldsymbol{n} \cdot \boldsymbol{\sigma} \equiv n_x\sigma_x + n_y\sigma_y + n_z\sigma_z$)

- Spin-1: $\hat{S}_x = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}$, $\hat{S}_y = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & -\mathbb{i} & 0 \\ \mathbb{i} & 0 & -\mathbb{i} \\ 0 & \mathbb{i} & 0 \end{pmatrix}$, $\hat{S}_z = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}$, under the $\hat{S}_z$ eigenbasis.

- The D_4 group: $\{(C_4)^{(n \mod 4)}(\sigma_s)^{(m \mod 2)} | C_4^4 = \sigma_s^2 = C_4\sigma_s C_4\sigma_s = \mathbb{1}\}$.

  8 elements, 5 conjugacy classes,

  $\{\mathbb{1}\}$, $\{C_4, C_4^3\}$, $\{C_4^2\}$, $\{\sigma_s, C_4^2\sigma_s\}$, and $\{C_4\sigma_s \equiv \sigma_d, C_4^3\sigma_s\}$.

  Character table for irreducible representations (irrep)

  $\Gamma_{1,2,3,4,5}$ is given on the right,

	$\mathbf{1}$	$2C_4$	C_4^2	$2\sigma_s$	$2\sigma_d$
Γ_1	1	1	1	1	1
Γ_2	1	1	1	−1	−1
Γ_3	1	−1	1	1	−1
Γ_4	1	−1	1	−1	1
Γ_5	2	0	−2	0	0

Problem 1. (20 points) Consider two spin-1 moments, $\hat{\boldsymbol{S}}_1$ and $\hat{\boldsymbol{S}}_2$. They satisfy $[\hat{S}_{i,a}, \hat{S}_{j,b}] = \delta_{i,j} \sum_c \mathrm{i}\epsilon^{abc} \hat{S}_{i,c}$ (here a, b, c label x, y, z components), and $\hat{\boldsymbol{S}}_1^2 = \hat{\boldsymbol{S}}_2^2 = 1 \cdot (1+1) = 2$. A complete orthonormal basis for the 9-dimensional Hilbert space is the $\hat{S}_z$ basis, $|s_1, s_2\rangle$. Here $s_i = 1, 0, -1$ are eigenvalues of $\hat{S}_{i,z}$ for $i = 1, 2$ respectively. The matrix elements of $\hat{S}_{i,a}$ for $i = 1, 2$ and $a = x, y, z$ are given on page 1.

(a) (10pts) *Write down the eigenvalues and normalized eigenstates (in terms of $\hat{S}_z$ basis) of $\hat{H}_0 = -J \cdot \hat{\boldsymbol{S}}_1 \cdot \hat{\boldsymbol{S}}_2$.* Here $J > 0$. [Hint: $\hat{H}_0$ is related to $(\hat{\boldsymbol{S}}_1 + \hat{\boldsymbol{S}}_2)^2$]

(b) (10pts) The full Hamiltonian is $\hat{H} = \hat{H}_0 + D \cdot [(\hat{S}_{1,z})^2 + (\hat{S}_{2,z})^2]$. D is a real "small" parameter. *Solve the energy eigenvalue(s) of the ground state(s) of $\hat{H}$ to second order of D.* [Hint: the unperturbed ground states of $\hat{H}_0$ are degenerate, but you may not need to use degenerate perturbation theory due to some symmetry]

Solution. This is similar to homework #6 Problem 1.

(a) This is the same as homework #6 Problem 1(a).

Define "total spin" $\hat{\boldsymbol{S}}_{1+2} = \hat{\boldsymbol{S}}_1 + \hat{\boldsymbol{S}}_2$. It's easy to check that different components of $\hat{\boldsymbol{S}}_{1+2}$ satisfy the commutation relations of angular momentum, and $[\hat{\boldsymbol{S}}_{1+2}^2, \hat{S}_{1+2,z}] = 0$. Define ladder operators $\hat{S}_{1+2,\pm} = \hat{S}_{1,\pm} + \hat{S}_{2,\pm}$.

$\hat{H}_0 = -\frac{J}{2}(\hat{\boldsymbol{S}}_1 + \hat{\boldsymbol{S}}_2)^2 + \frac{J}{2}(\hat{\boldsymbol{S}}_1)^2 + \frac{J}{2}(\hat{\boldsymbol{S}}_2)^2 = -\frac{J}{2}(\hat{\boldsymbol{S}}_1 + \hat{\boldsymbol{S}}_2)^2 + \frac{J}{2} \cdot 1 \cdot (1+1) + \frac{J}{2} \cdot 1 \cdot (1+1)$ $= -\frac{J}{2}(\hat{\boldsymbol{S}}_1 + \hat{\boldsymbol{S}}_2)^2 + 2J$. So the eigenstates of $\hat{H}_0$ can be chosen as the eigenstates of $\hat{\boldsymbol{S}}_{1+2}^2$ and $\hat{S}_{1+2,z}$, $|S_{1+2}, S_{1+2,z}\rangle$, with $S_{1+2} = 0$ or 1 or 2, and $S_{1+2,z} = -S_{1+2}, -S_{1+2}+1, \ldots, S_{1+2}$.

$|S_{1+2}, S_{1+2,z}\rangle$ are linear combinations of $|s_1, s_2\rangle$ with $s_1 + s_2 = S_{1+2,z}$.

For each S_{1+2}, first solve $|S_{1+2}, S_{1+2,z} = S_{1+2}\rangle$ in terms of $\hat{S}_z$ basis by the fact that $\hat{S}_{1+2,+}|S_{1+2}, S_{1+2,z} = S_{1+2}\rangle = 0$, then use the lowering ladder operator to generate other $S_{1+2,z}$ states.

$S_{1+2} = 2$ states are eigenstates of $\hat{H}_0$ with eigenvalue $-\frac{J}{2} \cdot 2 \cdot 3 + 2J = -J$,

$|S_{1+2} = 2, S_{1+2,z} = 2\rangle = |1, 1\rangle$;

$|S_{1+2} = 2, S_{1+2,z} = 1\rangle = \frac{S_{1+2,-}}{\sqrt{4}}|S_{1+2} = 2, S_{1+2,z} = 2\rangle = \frac{1}{\sqrt{2}}(|0, 1\rangle + |1, 0\rangle)$;

$|S_{1+2} = 2, S_{1+2,z} = 0\rangle = \frac{S_{1+2,-}}{\sqrt{6}}|S_{1+2} = 2, S_{1+2,z} = 1\rangle = \frac{1}{\sqrt{6}}(|-1, 1\rangle + 2|0, 0\rangle + |1, -1\rangle)$;

$|S_{1+2} = 2, S_{1+2,z} = -1\rangle = \frac{S_{1+2,-}}{\sqrt{6}}|S_{1+2} = 2, S_{1+2,z} = 0\rangle = \frac{1}{\sqrt{2}}(|-1, 0\rangle + |0, -1\rangle)$;

$|S_{1+2} = 2, S_{1+2,z} = -2\rangle = \frac{S_{1+2,-}}{\sqrt{4}}|S_{1+2} = 2, S_{1+2,z} = -1\rangle = |-1, -1\rangle$.

Suppose $|S_{1+2} = 1, S_{1+2,z} = 1\rangle = c_1|1,0\rangle + c_2|0,1\rangle$, then by $0 = \hat{S}_{1+2,+}|S_{1+2} = 1, S_{1+2,z} = 1\rangle = (\hat{S}_{1,+} + \hat{S}_{2,+})(c_1|1,0\rangle + c_2|0,1\rangle) = \sqrt{2}(c_1 + c_2)|1,1\rangle$, we have $c_2 = -c_1$. The normalized state $|S_{1+2} = 1, S_{1+2,z} = 1\rangle = \frac{1}{\sqrt{2}}(|1,0\rangle - |0,1\rangle)$.

$S_{1+2} = 1$ states are eigenstates of $\hat{H}_0$ with eigenvalue $-\frac{J}{2} \cdot 1 \cdot 2 + 2J = J$,
$|S_{1+2} = 1, S_{1+2,z} = 1\rangle = \frac{1}{\sqrt{2}}(|1,0\rangle - |0,1\rangle)$;
$|S_{1+2} = 1, S_{1+2,z} = 0\rangle = \frac{S_{1+2,-}}{\sqrt{2}}|S_{1+2} = 1, S_{1+2,z} = 1\rangle = \frac{1}{\sqrt{2}}(|1,-1\rangle - |0,-1\rangle)$;
$|S_{1+2} = 1, S_{1+2,z} = -1\rangle = \frac{S_{1+2,-}}{\sqrt{2}}|S_{1+2} = 1, S_{1+2,z} = 0\rangle = \frac{1}{\sqrt{2}}(|0,-1\rangle - |-1,0\rangle)$.

Suppose $|S_{1+2} = 0, S_{1+2,z} = 0\rangle = c_1|1,-1\rangle + c_2|0,0\rangle + c_3|-1,0\rangle$, then by $0 = \hat{S}_{1+2,+}|S_{1+2} = 0, S_{1+2,z} = 0\rangle = (\hat{S}_{1,+} + \hat{S}_{2,+})(c_1|1,-1\rangle + c_2|0,0\rangle + c_3|-1,0\rangle) = \sqrt{2}(c_1 + c_2)|1,0\rangle + \sqrt{2}(c_2 + c_3)|0,1\rangle$, we have $c_2 = -c_1$ and $c_3 = -c_2$. The normalized state $|S_{1+2} = 0, S_{1+2,z} = 0\rangle = \frac{1}{\sqrt{3}}(|1,-1\rangle - |0,0\rangle + |-1,1\rangle)$.

$S_{1+2} = 0$ states are eigenstates of $\hat{H}_0$ with eigenvalue $-\frac{J}{2} \cdot 0 \cdot 1 + 2J = 2J$,
$|S_{1+2} = 0, S_{1+2,z} = 0\rangle = \frac{1}{\sqrt{3}}(|1,-1\rangle - |0,0\rangle + |-1,1\rangle)$.

(b). This is similar to homework #6 Problem 1(b).

The full Hamiltonian $\hat{H}$ commutes with $\hat{S}_{1+2,z} = \hat{S}_{1,z} + \hat{S}_{2,z}$. Because $\hat{H}_0 = (-\frac{J}{2}\hat{\boldsymbol{S}}^2_{1+2} +$ constant) commutes with each component of $\hat{\boldsymbol{S}}_{1+2}$, and the perturbation $D \cdot (\hat{S}^2_{1,z} + \hat{S}^2_{2,z})$ commutes with both $\hat{S}_{1,z}$ and $\hat{S}_{2,z}$ according to the commutation relation given in main text of this problem.

The $\hat{S}_{1+2,z} = 2$ subspace has basis $|\hat{S}_{1+2} = 2, \hat{S}_{1+2,z} = 2\rangle$.

The $\hat{S}_{1+2,z} = 1$ subspace has basis $(|\hat{S}_{1+2} = 2, \hat{S}_{1+2,z} = 1\rangle, |\hat{S}_{1+2} = 1, \hat{S}_{1+2,z} = 1\rangle)$.

The $\hat{S}_{1+2,z} = 0$ subspace has basis $(|\hat{S}_{1+2} = 2, \hat{S}_{1+2,z} = 0\rangle, |\hat{S}_{1+2} = 1, \hat{S}_{1+2,z} = 0\rangle, |\hat{S}_{1+2} = 0, \hat{S}_{1+2,z} = 0\rangle)$.

The $\hat{S}_{1+2,z} = -1$ subspace has basis $(|\hat{S}_{1+2} = 2, \hat{S}_{1+2,z} = -1\rangle, |\hat{S}_{1+2} = 1, \hat{S}_{1+2,z} = -1\rangle)$.

The $\hat{S}_{1+2,z} = -2$ subspace has basis $|\hat{S}_{1+2} = 2, \hat{S}_{1+2,z} = -2\rangle$.

Under these basis choices, $\hat{H}_0$ is diagonal with diagonal elements being the eigenvalues in (a). The matrix elements of the perturbation term can be computed using the result of (a) about the $|S_{1+2}, S_{1+2,z}\rangle$ states. For example, $D \cdot (\hat{S}^2_{1,z} + \hat{S}^2_{2,z})|S_{1+2} = 2, S_{1+2,z} = 0\rangle$
$= D \cdot \frac{1}{\sqrt{6}}((1^2 + (-1)^2) \cdot |1,-1\rangle + (0^2 + 0^2) \cdot |0,0\rangle + ((-1)^2 + 1^2) \cdot |-1,1\rangle) = \frac{2D}{\sqrt{6}}(|1,-1\rangle + |-1,1\rangle)$
$= \frac{2D}{3}|S_{1+2} = 2, S_{1+2,z} = 0\rangle + \frac{2\sqrt{2}D}{3}|S_{1+2} = 0, S_{1+2,z} = 0\rangle$

The Hamiltonian matrices and (approximate) ground state energy in each subspace are given in the following table,

$S_{1+2,z}$	$\hat{H}_0 +$ perturbation	ground state energy
2	$(-J) + (2D)$	$= -J + 2D$
1	$\begin{pmatrix} -J & 0 \\ 0 & J \end{pmatrix} + \begin{pmatrix} D & 0 \\ 0 & D \end{pmatrix}$	$= -J + D$
0	$\begin{pmatrix} -J & 0 & 0 \\ 0 & J & 0 \\ 0 & 0 & 2J \end{pmatrix} + \begin{pmatrix} \frac{2D}{3} & 0 & \frac{2\sqrt{2}D}{3} \\ 0 & 2D & 0 \\ \frac{2\sqrt{2}D}{3} & 0 & \frac{4D}{3} \end{pmatrix}$	$\approx -J + \frac{2D}{3} + \frac{(2\sqrt{2}D/3)\cdot(\sqrt{2}D/3)}{(-J)-2J} = -J + \frac{2D}{3} - \frac{8D^2}{27}$
-1	$\begin{pmatrix} -J & 0 \\ 0 & J \end{pmatrix} + \begin{pmatrix} D & 0 \\ 0 & D \end{pmatrix}$	$= -J + D$
-2	$(-J) + (2D)$	$= -J + 2D$

The exact ground state energy in the $\hat{S}_{1+2,z} = 0$ space can be obtained by diagonalization of the 2×2 matrix $\begin{pmatrix} -J + \frac{2D}{3} & \frac{2\sqrt{2}D}{3} \\ \frac{2\sqrt{2}D}{3} & 2J + \frac{4D}{3} \end{pmatrix} = (\frac{J}{2} + D)\sigma_0 + \frac{2\sqrt{2}D}{3}\sigma_1 + (-\frac{3J}{2} - \frac{D}{3})\sigma_3$, and is $(\frac{J}{2} + D) - \sqrt{(\frac{2\sqrt{2}D}{3})^2 + (-\frac{3J}{2} - \frac{D}{3})^2} = (\frac{J}{2} + D) - (\frac{3J}{2} + \frac{D}{3}) \cdot \sqrt{1 + \frac{8D^2/9}{(3J/2+D/3)^2}}$
$\approx (\frac{J}{2} + D) - (\frac{3J}{2} + \frac{D}{3}) \cdot (1 + \frac{1}{2} \cdot \frac{8D^2/9}{9J^2/4}) \approx -J + \frac{2D}{3} - \frac{8D^2}{27J}$.

Problem 2. (30 points). Consider two fermion modes with annihilation operators denoted by $\hat{f}_i$ for $i = 1, 2$, satisfying $\{\hat{f}_i, \hat{f}_j^\dagger\} = \delta_{i,j}$ and $\{\hat{f}_i, \hat{f}_j\} = 0$. Denote the normalized vacuum state by $|\text{vac}\rangle$. The occupation basis states are $|\psi_0\rangle \equiv |\text{vac}\rangle$, $|\psi_1\rangle \equiv \hat{f}_1^\dagger|\text{vac}\rangle$, $|\psi_2\rangle \equiv \hat{f}_2^\dagger|\text{vac}\rangle$, and $|\psi_3\rangle \equiv \hat{f}_1^\dagger\hat{f}_2^\dagger|\text{vac}\rangle$. Let $\hat{H}_0 = E \cdot (\hat{n}_1 + \hat{n}_2)$, where E is a positive constant, $\hat{n}_i \equiv \hat{f}_i^\dagger\hat{f}_i$ are occupation number operators. Consider the Hamiltonian $\hat{H} = \hat{H}_0 + \Delta \cdot (\hat{f}_1^\dagger\hat{f}_2^\dagger + \hat{f}_2\hat{f}_1 + \hat{f}_1^\dagger\hat{f}_2^\dagger\hat{f}_2\hat{f}_1)$, where Δ is a real "small" parameter,

(a) (15pts) At time $t = 0$, set the initial state to $|\psi(t = 0)\rangle = |\psi_0\rangle = |\text{vac}\rangle$. Evolve this state by $\hat{H}$, namely $\mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t}|\psi(t)\rangle = \hat{H}|\psi(t)\rangle$. *Solve the transition probability to $|\psi_i\rangle$ state over time t, namely $|\langle\psi_i|\psi(t)\rangle|^2$, for $i = 1, 2, 3$, to lowest non-trivial order of Δ.* [Hint: use the interaction picture; note that $\hat{H}$ preserves particle number parity, decompose the Fock space into even- and odd-particle-number subspaces]

(b) (10pts) *Solve all eigenvalues of $\hat{H}$ up to cubic order of Δ.* [Hint: you don't have to use perturbation theory]

(c) (5pts) *Solve the transition probabilities defined in (a) exactly. Expand to lowest non-trivial order of Δ and compare with (a).* [Hint: some facts on page 1 may be useful]

Solution.

Rearrange the basis to $(|\psi_0\rangle, |\psi_3\rangle, |\psi_1\rangle, |\psi_2\rangle)$.

$\hat{H}$ is the following block-diagonal matrix, $\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 2E & 0 & 0 \\ 0 & 0 & E & 0 \\ 0 & 0 & 0 & E \end{pmatrix} + \begin{pmatrix} 0 & \Delta & 0 & 0 \\ \Delta & \Delta & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$.

Because it preserves total-particle-number parity, so does not have matrix element between even-particle-number states ($|\psi_{0,3}\rangle$) and odd-particle-number states ($|\psi_{1,2}\rangle$).

The steps for computing these matrix elements are omitted here.

(a). Because $\hat{H}$ is independent of time, $|\psi(t)\rangle = \exp(-\frac{\mathbb{i}}{\hbar}\hat{H}\cdot t)|\psi(t=0)\rangle$.

Use the interaction picture, define $\hat{U}_I(t) = \exp(\frac{\mathbb{i}}{\hbar}\hat{H}_0\cdot t)\cdot\exp(-\frac{\mathbb{i}}{\hbar}\hat{H}\cdot t)$. Then $\mathbb{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t}\hat{U}_I(t) = \hat{V}_I(t)\hat{U}_I(t)$, where $\hat{V}_I(t) \equiv \exp(\frac{\mathbb{i}}{\hbar}\hat{H}_0\cdot t)\cdot\hat{V}_S\cdot\exp(-\frac{\mathbb{i}}{\hbar}\hat{H}_0\cdot t)$, and the Schrödinger picture perturbation operator $\hat{V}_S$ is $\hat{V}_S \equiv \Delta\cdot(\hat{f}_1^\dagger\hat{f}_2^\dagger + \hat{f}_2\hat{f}_1 + \hat{f}_1^\dagger\hat{f}_2^\dagger\hat{f}_2\hat{f}_1)$. The Dyson series form of $\hat{U}_I$ is $\hat{U}_I(t) = \mathbb{1} + \frac{-\mathbb{i}}{\hbar}\int_0^t \mathrm{d}t_1\,\hat{V}_I(t_1) + (\frac{-\mathbb{i}}{\hbar})^2\int_0^t \mathrm{d}t_1\int_0^{t_1}\mathrm{d}t_2\,\hat{V}_I(t_1)\hat{V}_I(t_1) + \ldots$.

Note that $|\psi_i\rangle$ are eigenstates of $\hat{H}_0$ with eigenvalue $E_i = 0, E, E, 2E$ for $i = 1,2,3,4$ respectively. Then $|\langle\psi_i|\psi(t)\rangle|^2 = |\langle\psi_i|e^{-\mathbb{i}\hat{H}_0\cdot t/\hbar}\hat{U}_I(t)|\psi_0\rangle|^2 = |\langle\psi_i|e^{-\mathbb{i}E_i\cdot t/\hbar}\hat{U}_I(t)|\psi_0\rangle|^2 = |\langle\psi_i|\hat{U}_I(t)|\psi_0\rangle|^2$.

Under the $(|\psi_0\rangle, |\psi_3\rangle, |\psi_1\rangle, |\psi_2\rangle)$ basis, $\hat{V}_I(t)$ is $\begin{pmatrix} 0 & \Delta e^{-\frac{\mathbb{i}}{\hbar}2E\cdot t} & 0 & 0 \\ \Delta e^{\frac{\mathbb{i}}{\hbar}2E\cdot t} & \Delta & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$.

Combine this with the Dyson series form of $\hat{U}_I$, it is easy to see that $\langle\psi_1|\hat{U}_I(t)|\psi_0\rangle = \langle\psi_2|\hat{U}_I(t)|\psi_0\rangle = 0$ to all orders of perturbation, because $\langle\psi_{1,2}|\hat{V}_I(t) = 0$.

To lowest non-trivial order, $\langle\psi_3|\hat{U}_I(t)|\psi_0\rangle \approx 0 + \frac{-\mathbb{i}}{\hbar}\int_0^t\langle\psi_3|\hat{V}_I(t_1)|\psi_0\rangle$
$= 0 + \frac{-\mathbb{i}}{\hbar}\int_0^t \mathrm{d}t_1\,\Delta e^{\frac{\mathbb{i}}{\hbar}2E\cdot t_1} = -\frac{\Delta}{2E}\cdot(e^{\frac{\mathbb{i}}{\hbar}2E\cdot t} - 1) = -\mathbb{i}e^{\mathbb{i}\frac{E\cdot t}{\hbar}}\frac{\Delta}{E}\sin(\frac{E\cdot t}{\hbar})$.

Finally $|\langle\psi_1|\psi(t)\rangle|^2 = 0$, $|\langle\psi_2|\psi(t)\rangle|^2 = 0$, $|\langle\psi_3|\psi(t)\rangle|^2 \approx [\frac{\Delta}{E}\sin(\frac{E\cdot t}{\hbar})]^2$.

(b) From the matrix form of $\hat{H}$, it is easy to see that $|\psi_1\rangle$ and $|\psi_2\rangle$ are already eigenstates of perturbed Hamiltonian $\hat{H}$ with eigenvalue E.

In the subspace spanned by $(|\psi_0\rangle, |\psi_3\rangle)$, $\hat{H}$ is a 2×2 matrix, $\begin{pmatrix} 0 & 0 \\ 0 & 2E \end{pmatrix} + \begin{pmatrix} 0 & \Delta \\ \Delta & \Delta \end{pmatrix}$ $(E+\frac{\Delta}{2})\sigma_0 + (-E-\frac{\Delta}{2})\sigma_3 + \Delta\sigma_1$. Perturbation theory can be used, but the exact eigenvalues can also be easily computed. The eigenvalues are [see homework #1 Problem 4(a)],

$(E+\frac{\Delta}{2}) \pm \sqrt{(-E-\frac{\Delta}{2})^2+\Delta^2} = (E+\frac{\Delta}{2}) \pm (E+\frac{\Delta}{2})\sqrt{1+\frac{\Delta^2}{(E+\Delta/2)^2}}$

$\approx (E+\frac{\Delta}{2}) \pm (E+\frac{\Delta}{2})\cdot[1+\frac{1}{2}\cdot\frac{\Delta^2}{(E+\Delta/2)^2}+O(\Delta^4)]$

$\approx (E+\frac{\Delta}{2}) \pm \left[(E+\frac{\Delta}{2})+\frac{1}{2}\frac{\Delta^2}{E}(1-\frac{\Delta}{2E})\right]+O(\Delta^4)$,

where $O(\Delta^4)$ means terms of 4th or higher orders.

You can also use $\sqrt{1+x}\approx 1+\frac{x}{2}-\frac{x^2}{8}+\frac{x^3}{16}+O(x^4)$ to do the expansion,

$\sqrt{(-E-\frac{\Delta}{2})^2+\Delta^2} = E\cdot\sqrt{1+(\frac{\Delta}{E}+\frac{5}{4}\frac{\Delta^2}{E^2})}$

$\approx E\cdot\left[1+\frac{1}{2}\cdot(\frac{\Delta}{E}+\frac{5}{4}\frac{\Delta^2}{E^2})-\frac{1}{8}\cdot(\frac{\Delta}{E}+\frac{5}{4}\frac{\Delta^2}{E^2})^2+\frac{1}{16}\cdot(\frac{\Delta}{E}+\frac{5}{4}\frac{\Delta^2}{E^2})^3\right]+O(\Delta^4)$

$\approx E\cdot\left[1+(\frac{1}{2}\frac{\Delta}{E}+\frac{5}{8}\frac{\Delta^2}{E^2})-(\frac{1}{8}\frac{\Delta^2}{E^2}+\frac{5}{16}\frac{\Delta^3}{E^3})+\frac{1}{16}\frac{\Delta^3}{E^3}\right]+O(\Delta^4)$

$= E+\frac{\Delta}{2}+\frac{\Delta^2}{2E}-\frac{\Delta^3}{4E^2}+O(\Delta^4)$.

Finally, the approximate eigenvalues are E, E, $-\frac{\Delta^2}{2E}+\frac{\Delta^3}{4E^2}$, and $2E+\Delta+\frac{\Delta^2}{2E}-\frac{\Delta^3}{4E^2}$.

(c) The time-evolution operator $\exp(-\frac{\mathrm{i}}{\hbar}\hat{H}\cdot t)$ can be computed exactly.

Under the previous basis, it has the following block diagonal form,

$$\begin{pmatrix} \exp\left[-\frac{\mathrm{i}}{\hbar}\begin{pmatrix} 0 & \Delta \\ \Delta & 2E+\Delta \end{pmatrix}\cdot t\right] & 0_{2\times 2} \\ 0_{2\times 2} & e^{-\frac{\mathrm{i}}{\hbar}E\cdot t}\mathbb{1}_{2\times 2} \end{pmatrix}.$$

Then obviously $\langle\psi_{1,2}|\exp(-\frac{\mathrm{i}}{\hbar}\hat{H}\cdot t)|\psi_0\rangle = 0$.

Use the facts on page 1 [also in homework #1 Problem 4(b)],

$\exp\left[-\frac{\mathrm{i}}{\hbar}\begin{pmatrix} 0 & \Delta \\ \Delta & 2E+\Delta \end{pmatrix}\cdot t\right] = \exp[-\mathrm{i}\frac{t}{\hbar}((E+\frac{\Delta}{2})\sigma_0+(-E-\frac{\Delta}{2})\sigma_3+\Delta\sigma_1)]$

$= e^{-\mathrm{i}\frac{(E+\Delta/2)}{\hbar}t}\cdot[\cos(\omega\cdot t)\sigma_0 - \mathrm{i}\sin(\omega\cdot t)(\frac{-E-\Delta/2}{\omega}\sigma_3+\frac{\Delta}{\omega}\sigma_1)]$,

where $\omega = \sqrt{(-E-\Delta/2)^2+\Delta^2} = \sqrt{E^2+E\Delta+5\Delta^2/4}$.

Therefore $\langle\psi_3|\exp(-\frac{\mathrm{i}}{\hbar}\hat{H}\cdot t)|\psi_0\rangle = -e^{-\mathrm{i}\frac{(E+\Delta/2)}{\hbar}t}\cdot\mathrm{i}\sin(\omega\cdot t)\cdot\frac{\Delta}{\omega}$.

Finally the exact transition probabilities are

$|\langle\psi_1|\psi(t)\rangle|^2 = 0$, $|\langle\psi_2|\psi(t)\rangle|^2 = 0$, $|\langle\psi_3|\psi(t)\rangle|^2 = [\frac{\Delta}{\omega}\sin(\omega\cdot t)]^2$.

To lowest order approximation $\omega\approx E$, this reduces to the result of (a).

Problem 4. (40 points) Consider four spin-1/2 moments, labeled by subscripts $_i$ with $i = 1, 2, 3, 4$ respectively. Denote the tensor product of $\hat{S}_z$ eigenbasis by $|s_1, s_2, s_3, s_4\rangle$, where $s_i = \pm\frac{1}{2}$ is the eigenvalue of $\hat{S}_{i,z}$. For simplicity, denote $s_i = +\frac{1}{2}$ by $\uparrow$, and $s_i = -\frac{1}{2}$ by $\downarrow$. The commutation relation of the spin operators is $[\hat{S}_{i,a}, \hat{S}_{j,b}] = \delta_{i,j}\mathbb{i}\sum_c \epsilon^{abc}\hat{S}_{i,c}$.

(a). (4pts) *Show that the following four hermitian operators mutually commute,* $(\hat{\boldsymbol{S}}_1 + \hat{\boldsymbol{S}}_2 + \hat{\boldsymbol{S}}_3 + \hat{\boldsymbol{S}}_4)^2$, $(\hat{S}_{1,z} + \hat{S}_{2,z} + \hat{S}_{3,z} + \hat{S}_{4,z})$, $(\hat{\boldsymbol{S}}_1 + \hat{\boldsymbol{S}}_3)^2$, $(\hat{\boldsymbol{S}}_2 + \hat{\boldsymbol{S}}_4)^2$.

(b). (16pts) Suppose the four operators in (a) have the following simultaneous eigenvalues, $S(S+1)$, S_z, $S_{1+3}(S_{1+3}+1)$, $S_{2+4}(S_{2+4}+1)$, respectively. *Find the possible combinations of these "quantum numbers", and the normalized eigenstates $|S, S_z, S_{1+3}, S_{2+4}\rangle$ in terms of $\hat{S}_z$ basis.* [Hint: add the spins '1' and '3' first, solve $|S_{1+3}, S_{1+3,z}\rangle$ in terms of $|s_1, s_3\rangle$; add the spins '2' and '4' in similar fashion; then make linear combinations of $|S_{1+3}, S_{1+3,z}\rangle|S_{2+4}, S_{2+4,z}\rangle$, the results of some previous problem may help]

(c). (4pts) *Solve the eigenvalues of $\hat{H} = \hat{\boldsymbol{S}}_1 \cdot \hat{\boldsymbol{S}}_2 + \hat{\boldsymbol{S}}_2 \cdot \hat{\boldsymbol{S}}_3 + \hat{\boldsymbol{S}}_3 \cdot \hat{\boldsymbol{S}}_4 + \hat{\boldsymbol{S}}_4 \cdot \hat{\boldsymbol{S}}_1$.* [Hint: try to relate $\hat{H}$ with the operators in (a), then use the result of (b)]

(d). (16pts) Consider the D_4 group (see page 1) generated by
$C_4 : \ |s_1, s_2, s_3, s_4\rangle \mapsto |s_4, s_1, s_2, s_3\rangle$; and $\sigma_s : \ |s_1, s_2, s_3, s_4\rangle \mapsto |s_1, s_4, s_3, s_2\rangle$.
The D_4 group elements commute with the total spin operators $\sum_{i=1}^{4} \hat{\boldsymbol{S}}_i$. We can construct complete orthonormal basis states of D_4 irreducible representations(irrep), labeled by $|S, S_z, (\Gamma_i, j)\rangle$. S and S_z are defined in (b). $i = 1, 2, 3, 4, 5$ label the type of irrep. $j = 1, 2$ for the 2-dimensional Γ_5 irrep, label the two basis states of a Γ_5 irrep; and $j = 1$ (can be omitted) for other 1-dimensional irrep. Under the action of group generators, these states transform as $C_4 : \ |S, S_z, (\Gamma_i, j)\rangle \mapsto \sum_{j'} |S, S_z, (\Gamma_i, j')\rangle \cdot [R_{\Gamma_i}(C_4)]_{j',j}$; and
$\sigma_s : \ |S, S_z, (\Gamma_i, j)\rangle \mapsto \sum_{j'} |S, S_z, (\Gamma_i, j')\rangle \cdot [R_{\Gamma_i}(\sigma_s)]_{j',j}$. Here $R_{\Gamma_i}(g)$ is the representation matrix (1×1 for $\Gamma_{1,2,3,4}$, 2×2 for Γ_5) for group element g. *Construct these $|S, S_z, (\Gamma_i, j)\rangle$ states in terms of $\hat{S}_z$ eigenbasis. And write down the representation matrices $R_{\Gamma_i}(C_4)$ and $R_{\Gamma_i}(\sigma_s)$ under these basis.* [Hint:
method #1: use the basis in (b), figure out how they transform under the group generators, and (if necessary) make linear combinations to form irreducible represen-

tations, $|S,S_z,(\Gamma_i,j)\rangle = \sum_{S_{1+3}}\sum_{S_{2+4}}|S,S_z,S_{1+3},S_{2+4}\rangle\langle S,S_z,S_{1+3},S_{2+4}|S,S_z,(\Gamma_i,j)\rangle$, because the D_4 group elements commute with ladder operators, the coefficients $\langle S,S_z,S_{1+3},S_{2+4}|S,S_z,(\Gamma_i,j)\rangle$ is independent of S_z, so you only need to work out these coefficients for highest $S_z = S$ by *e.g.* "projection operator";
method #2: use the "projection operator" on the $|s_1,s_2,s_3,s_4\rangle$ basis directly in each total S_z subspace, and compare the results to (b) to figure out the S quantum number, you may need to make linear combinations of states with the same S_z and the same irrep]

Solution.

(a). Define $\hat{\boldsymbol{S}}_{1+3} = \hat{\boldsymbol{S}}_1 + \hat{\boldsymbol{S}}_3$, $\hat{\boldsymbol{S}}_{2+4} = \hat{\boldsymbol{S}}_2 + \hat{\boldsymbol{S}}_4$, and $\hat{\boldsymbol{S}} = \hat{\boldsymbol{S}}_1 + \hat{\boldsymbol{S}}_2 + \hat{\boldsymbol{S}}_3 + \hat{\boldsymbol{S}}_4 = \hat{\boldsymbol{S}}_{1+3} + \hat{\boldsymbol{S}}_{2+4}$. The fact that these four operators commute has been used in the "addition of angular momentum".

Components of $\hat{\boldsymbol{S}}$ satisfy the commutation relation of angular momentum, $[\hat{S}_a,\hat{S}_b] = \mathbb{i}\sum_c \epsilon^{abc}\hat{S}_c$. Then $[\hat{\boldsymbol{S}}^2,\hat{S}_z] = [\hat{S}_x^2+\hat{S}_y^2,\hat{S}_z]+0 = [\hat{S}_x,\hat{S}_z]\hat{S}_x+\hat{S}_x[\hat{S}_x,\hat{S}_z]+[\hat{S}_y,\hat{S}_z]\hat{S}_y+\hat{S}_y[\hat{S}_y,\hat{S}_z] = -\mathbb{i}\hat{S}_y\cdot\hat{S}_x + \hat{S}_x\cdot(-\mathbb{i}\hat{S}_y) + \mathbb{i}\hat{S}_x\cdot\hat{S}_y + \hat{S}_y\cdot\mathbb{i}\hat{S}_x = 0$.

Similarly we have $[\hat{\boldsymbol{S}}^2_{1+3},\hat{S}_{1+3,a}] = 0$ and $[\hat{\boldsymbol{S}}^2_{2+4},\hat{S}_{2+4,a}] = 0$, for $a = x,y,z$.

It is obvious that $[\hat{\boldsymbol{S}}^2_{1+3},\hat{\boldsymbol{S}}^2_{2+4}] = 0$, and $[\hat{\boldsymbol{S}}^2_{2+4},\hat{S}_{1+3,a}] = 0$ and $[\hat{\boldsymbol{S}}^2_{1+3},\hat{S}_{2+4,a}] = 0$ for $a = x,y,z$. Because the two operators in the commutator do not share spin operators of the same spin.

Then $[\hat{\boldsymbol{S}}^2_{2+4},\hat{S}_z] = [\hat{\boldsymbol{S}}^2_{2+4},\hat{S}_{1+3,z}+\hat{S}_{2+4,z}] = 0$, and $[\hat{\boldsymbol{S}}^2_{1+3},\hat{S}_z] = [\hat{\boldsymbol{S}}^2_{1+3},\hat{S}_{1+3,z}+\hat{S}_{2+4,z}] = 0$.

Finally $\hat{\boldsymbol{S}}_{1+3}\cdot\hat{\boldsymbol{S}}_{2+4} = \sum_a \hat{S}_{1+3,a}\cdot\hat{S}_{2+4,a}$ commutes with $\hat{\boldsymbol{S}}^2_{1+3}$ and $\hat{\boldsymbol{S}}^2_{2+4}$, because the factors $\hat{S}_{1+3,a}$ and $\hat{S}_{2+4,a}$ commute with $\hat{\boldsymbol{S}}^2_{1+3}$ and $\hat{\boldsymbol{S}}^2_{2+4}$. And consider $\hat{\boldsymbol{S}}^2 = \hat{\boldsymbol{S}}^2_{1+3} + \hat{\boldsymbol{S}}^2_{2+4} + 2\hat{\boldsymbol{S}}_{1+3}\cdot\hat{\boldsymbol{S}}_{2+4}$. We have $[\hat{\boldsymbol{S}}^2,\hat{\boldsymbol{S}}^2_{1+3}] = 0$, and $[\hat{\boldsymbol{S}}^2,\hat{\boldsymbol{S}}^2_{2+4}] = 0$.

(b) Compose $|S_{1+3},S_{1+3,z}\rangle$ states in terms of $|s_1,s_3\rangle$. This is the same as homework #5 Problem 1(a). S_{1+3} can be 1 or 0, $\boldsymbol{\frac{1}{2}}\otimes\boldsymbol{\frac{1}{2}} = \mathbf{1}\oplus\mathbf{0}$.

$|S_{1+3}=1,S_{1+3,z}=1\rangle = |\uparrow\uparrow\rangle$,

$|S_{1+3}=1,S_{1+3,z}=0\rangle = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)$,

$|S_{1+3}=1,S_{1+3,z}=-1\rangle = |\downarrow\downarrow\rangle$.

$|S_{1+3}=0,S_{1+3,z}=0\rangle = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$.

The $|S_{2+4},S_{2+4,z}\rangle$ states in terms of $|s_2,s_4\rangle$ have exactly the same form. Finally compose $|S,S_z,S_{1+3},S_{2+4}\rangle$ in terms of $|S_{1+3},S_{1+3,z}\rangle|S_{2+4},S_{2+4,z}\rangle$. Note $|s_1,s_3\rangle|s_2,s_4\rangle = |s_1,s_2,s_3,s_4\rangle$.

If $S_{1+3}=0$ and $S_{2+4}=0$, then S must be 0,

$|S=0,S_z=0,S_{1+3}=0,S_{2+4}=0\rangle=|S_{1+3}=0,S_{1+3,z}=0\rangle|S_{2+4}=0,S_{2+4,z}=0\rangle$
$=\frac{1}{2}(|\uparrow\uparrow\downarrow\downarrow\rangle-|\uparrow\downarrow\downarrow\uparrow\rangle-|\downarrow\uparrow\uparrow\downarrow\rangle+|\downarrow\downarrow\uparrow\uparrow\rangle)$.

If $S_{1+3}=1$ and $S_{2+4}=0$, then S must be 1,

$|S=1,S_z=1,S_{1+3}=1,S_{2+4}=0\rangle=|S_{1+3}=1,S_{1+3,z}=1\rangle|S_{2+4}=0,S_{2+4,z}=0\rangle$
$=\frac{1}{\sqrt{2}}(|\uparrow\uparrow\uparrow\downarrow\rangle-|\uparrow\downarrow\uparrow\uparrow\rangle)$,
$|S=1,S_z=0,S_{1+3}=1,S_{2+4}=0\rangle=|S_{1+3}=1,S_{1+3,z}=0\rangle|S_{2+4}=0,S_{2+4,z}=0\rangle$
$=\frac{1}{2}(|\uparrow\uparrow\downarrow\downarrow\rangle-|\uparrow\downarrow\downarrow\uparrow\rangle+|\downarrow\uparrow\uparrow\downarrow\rangle-|\downarrow\downarrow\uparrow\uparrow\rangle)$,
$|S=1,S_z=-1,S_{1+3}=1,S_{2+4}=0\rangle=|S_{1+3}=1,S_{1+3,z}=-1\rangle|S_{2+4}=0,S_{2+4,z}=0\rangle$
$=\frac{1}{\sqrt{2}}(|\downarrow\uparrow\downarrow\downarrow\rangle-|\downarrow\downarrow\downarrow\uparrow\rangle)$.

If $S_{1+3}=0$ and $S_{2+4}=1$, then S must be 1,

$|S=1,S_z=1,S_{1+3}=0,S_{2+4}=1\rangle=|S_{1+3}=0,S_{1+3,z}=0\rangle|S_{2+4}=1,S_{2+4,z}=1\rangle$
$=\frac{1}{\sqrt{2}}(|\uparrow\uparrow\downarrow\uparrow\rangle-|\downarrow\uparrow\uparrow\uparrow\rangle)$,
$|S=1,S_z=0,S_{1+3}=0,S_{2+4}=1\rangle=|S_{1+3}=0,S_{1+3,z}=0\rangle|S_{2+4}=1,S_{2+4,z}=0\rangle$
$=\frac{1}{2}(|\uparrow\uparrow\downarrow\downarrow\rangle+|\uparrow\downarrow\downarrow\uparrow\rangle-|\downarrow\uparrow\uparrow\downarrow\rangle-|\downarrow\downarrow\uparrow\uparrow\rangle)$,
$|S=1,S_z=-1,S_{1+3}=0,S_{2+4}=1\rangle=|S_{1+3}=0,S_{1+3,z}=0\rangle|S_{2+4}=1,S_{2+4,z}=-1\rangle$
$=\frac{1}{\sqrt{2}}(|\uparrow\downarrow\downarrow\downarrow\rangle-|\downarrow\downarrow\uparrow\downarrow\rangle)$.

If $\hat{S}_{1+3}=1$ and $S_{2+4}=1$, then S can be 2 or 1 or 0, this part is exactly the same as problem 1(a), just replace the $|s_1,s_2\rangle$ basis there by $|S_{1+3},S_{1+3,z}=s_1\rangle|S_{2+4},S_{2+4,z}=s_2\rangle$,

$|S=2,S_z=2,S_{1+3}=1,S_{2+4}=1\rangle=|\uparrow\uparrow\uparrow\uparrow\rangle$,
$|S=2,S_z=1,S_{1+3}=1,S_{2+4}=1\rangle=\frac{1}{2}(|\uparrow\uparrow\downarrow\uparrow\rangle+|\downarrow\uparrow\uparrow\uparrow\rangle+|\uparrow\uparrow\uparrow\downarrow\rangle+|\uparrow\downarrow\uparrow\uparrow\rangle)$,
$|S=2,S_z=0,S_{1+3}=1,S_{2+4}=1\rangle$
$=\frac{1}{\sqrt{6}}(|\downarrow\uparrow\downarrow\uparrow\rangle+|\uparrow\uparrow\downarrow\downarrow\rangle+|\uparrow\downarrow\downarrow\uparrow\rangle+|\downarrow\uparrow\uparrow\downarrow\rangle+|\downarrow\downarrow\uparrow\uparrow\rangle+|\uparrow\downarrow\uparrow\downarrow\rangle)$,
$|S=2,S_z=1,S_{1+3}=-1,S_{2+4}=1\rangle=\frac{1}{2}(|\downarrow\uparrow\downarrow\downarrow\rangle+|\downarrow\downarrow\downarrow\uparrow\rangle+|\uparrow\downarrow\downarrow\downarrow\rangle+|\downarrow\downarrow\uparrow\downarrow\rangle)$,
$|S=2,S_z=-2,S_{1+3}=1,S_{2+4}=1\rangle=|\downarrow\downarrow\downarrow\downarrow\rangle$.

$|S=1,S_z=1,S_{1+3}=1,S_{2+4}=1\rangle=\frac{1}{2}(|\uparrow\uparrow\uparrow\downarrow\rangle+|\uparrow\downarrow\uparrow\uparrow\rangle-|\uparrow\uparrow\downarrow\uparrow\rangle-|\downarrow\uparrow\uparrow\uparrow\rangle)$,
$|S=1,S_z=0,S_{1+3}=1,S_{2+4}=1\rangle=\frac{1}{\sqrt{2}}(|\uparrow\downarrow\uparrow\downarrow\rangle-|\downarrow\uparrow\downarrow\uparrow\rangle)$,
$|S=1,S_z=-1,S_{1+3}=1,S_{2+4}=1\rangle=\frac{1}{2}(|\uparrow\downarrow\downarrow\downarrow\rangle+|\downarrow\downarrow\uparrow\downarrow\rangle-|\downarrow\uparrow\downarrow\downarrow\rangle-|\downarrow\downarrow\downarrow\uparrow\rangle)$,

$|S=0,S_z=0,S_{1+3}=1,S_{2+4}=1\rangle$
$=\frac{1}{2\sqrt{3}}(2|\uparrow\downarrow\uparrow\downarrow\rangle-|\uparrow\uparrow\downarrow\downarrow\rangle-|\uparrow\downarrow\downarrow\uparrow\rangle-|\downarrow\uparrow\uparrow\downarrow\rangle-|\downarrow\downarrow\uparrow\uparrow\rangle+2|\downarrow\uparrow\downarrow\uparrow\rangle)$.

(c) $\hat{H} = (\hat{\boldsymbol{S}}_1 + \hat{\boldsymbol{S}}_3) \cdot (\hat{\boldsymbol{S}}_2 + \hat{\boldsymbol{S}}_4) = \frac{1}{2}[(\hat{\boldsymbol{S}}_1 + \hat{\boldsymbol{S}}_2 + \hat{\boldsymbol{S}}_3 + \hat{\boldsymbol{S}}_4)^2 - (\hat{\boldsymbol{S}}_1 + \hat{\boldsymbol{S}}_3)^2 - (\hat{\boldsymbol{S}}_2 + \hat{\boldsymbol{S}}_4)^2]$.

Therefore the $|S, S_z, S_{1+3}, S_{2+4}\rangle$ states in (b) are eigenstates of $\hat{H}$ with eigenvalues $\frac{1}{2}[S(S+1) - S_{1+3}(S_{1+3}+1) - S_{2+4}(S_{2+4}+1)]$. These are summarized in the following table,

S	S_z	S_{1+3}	S_{2+4}	H eigenvalue
0	$0,$	0	0	0
1	$1, 0, -1,$	1	0	0
1	$1, 0, -1,$	0	1	0
2	$2, 1, 0, -1, -2,$	1	1	1
1	$1, 0, -1,$	1	1	-1
0	$0,$	1	1	-2

(d) This is similar to homework #5 Problem 1(c).

Use the method #1 in the Hint, and the following hint given during the exam.

Because the D_4 group elements commute with $\hat{\boldsymbol{S}}$ operators, and in particular commute with the ladder operators. The action of group elements do not change S and S_z quantum numbers, but may change S_{1+3} and S_{2+4}.

If the action of group element g on highest $S_z = S$ states is
$|S, S_z = S, S_{1+3}, S_{2+4}\rangle \mapsto \sum_{S'_{1+3}, S'_{2+4}} |S, S_z = S, S'_{1+3}, S'_{2+4}\rangle \cdot [R(g)]_{(S'_{1+3}, S'_{2+4}),(S_{1+3}, S_{2+4})}$,
where $R(g)$ is the representation matrix the combination (S'_{1+3}, S'_{2+4}) is the row index and (S_{1+3}, S_{2+4}) is the column index, then this representation matrix is independent of S_z,
$|S, S_z, S_{1+3}, S_{2+4}\rangle \mapsto \sum_{S'_{1+3}, S'_{2+4}} |S, S_z, S'_{1+3}, S'_{2+4}\rangle \cdot [R(g)]_{(S'_{1+3}, S'_{2+4}),(S_{1+3}, S_{2+4})}$.
Because S_z can be changed by application of lowering ladder operator $\hat{S}_- = \sum_{i=1}^4 \hat{S}_{i,-}$.

So we only need to work out the $R(g)$ matrices for each subspace with certain S and $S_z = S$. This can be done by the definition of C_4 and σ_s in the $|s_1, s_2, s_3, s_4\rangle$ basis, and the result of (b). The results are

basis	$R(C_4)$	$R(\sigma_s)$
$\|S=0, S_z=0, S_{1+3}=0, S_{2+4}=0\rangle$	(-1)	(-1)
$(\|S=1, S_z=1, S_{1+3}=1, S_{2+4}=0\rangle,$ $\|S=1, S_z=1, S_{1+3}=0, S_{2+4}=1\rangle)$	$\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$	$\begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}$
$\|S=0, S_z=0, S_{1+3}=1, S_{2+4}=1\rangle$	(1)	(1)
$\|S=1, S_z=1, S_{1+3}=1, S_{2+4}=1\rangle$	(-1)	(1)
$\|S=2, S_z=2, S_{1+3}=1, S_{2+4}=1\rangle$	(1)	(1)

These are already irreducible representations. So the $|S, S_z, (\Gamma_i, j)\rangle$ basis are

$\|S, S_z, (\Gamma_i, j)\rangle$ states	in terms of $\|S, S_z, S_{1+3}, S_{2+4}\rangle$	$R(C_4)$	$R(\sigma_s)$
$\|S=0, S_z, (\Gamma_4, j=1)\rangle$	$\|S=0, S_z, S_{1+3}=0, S_{2+4}=0\rangle$	(-1)	(-1)
$\|S=1, S_z, (\Gamma_5, j=1)\rangle$	$\|S=1, S_z, S_{1+3}=1, S_{2+4}=0\rangle$	$\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$	$\begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}$
$\|S=1, S_z, (\Gamma_5, j=2)\rangle$	$\|S=1, S_z, S_{1+3}=0, S_{2+4}=1\rangle$		
$\|S=0, S_z, (\Gamma_1, j=1)\rangle$	$\|S=0, S_z, S_{1+3}=1, S_{2+4}=1\rangle$	(1)	(1)
$\|S=1, S_z, (\Gamma_3, j=1)\rangle$	$\|S=1, S_z, S_{1+3}=1, S_{2+4}=1\rangle$	(-1)	(1)
$\|S=2, S_z, (\Gamma_1, j=1)\rangle$	$\|S=2, S_z, S_{1+3}=1, S_{2+4}=1\rangle$	(1)	(1)

Here S_z can be $-S, -S+1, \dots, S$.

The choice of Γ_5 basis are of course not unique.

If you use method #2 in the Hint, you will eventually get the same result. But the "projection operator" results for Γ_1 irrep in the $S_z = 0$ subspace are

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

$= \sqrt{\frac{2}{3}}|S=2, S_z=0, S_{1+3}=1, S_{2+4}=1\rangle - \sqrt{\frac{1}{3}}|S=0, S_z=0, S_{1+3}=1, S_{2+4}=1\rangle$, and

$\frac{1}{\sqrt{2}}(|\uparrow\downarrow\uparrow\downarrow\rangle + |\downarrow\uparrow\downarrow\uparrow\rangle)$

$= \sqrt{\frac{1}{3}}|S=2, S_z=0, S_{1+3}=1, S_{2+4}=1\rangle + \sqrt{\frac{2}{3}}|S=0, S_z=0, S_{1+3}=1, S_{2+4}=1\rangle$.

You need to make linear combinations of these to get total-S eigenstates.

Problem 5. (10 points) ("Heisenberg chain") Consider N spin-1/2 moments labeled by subscripts $_i$ with $i = 0, 1, \dots, (N-1)$. Here N is a large integer. The 1D Heisenberg model Hamiltonian is $\hat{H} = -J\sum_{i=0}^{N-1}(\hat{\boldsymbol{S}}_i \cdot \hat{\boldsymbol{S}}_{i+1} - \frac{1}{4})$. Here we assume periodic boundary condition, so $\hat{\boldsymbol{S}}_N$ is actually $\hat{\boldsymbol{S}}_0$. From $\hat{\boldsymbol{S}}_i \cdot \hat{\boldsymbol{S}}_{i+1} = \hat{S}_{i,z}\hat{S}_{i+1,z} + \frac{1}{2}(\hat{S}_{i,+}\hat{S}_{i+1,-} + \hat{S}_{i,-}\hat{S}_{i+1,+})$, it is easy to see that the fully polarized state, $|\downarrow\downarrow\dots\downarrow\rangle$, is an eigenstate of $\hat{H}$ with eigenvalue (0). Label the other $\hat{S}_z$ eigenstates by the positions of $\uparrow$, for example $|x\rangle \equiv \hat{S}_{x,+}|\downarrow\downarrow\dots\downarrow\rangle$ has one $\uparrow$ at position $x = 0, 1, \dots, (N-1)$.

The lattice translation, $\hat{T} : |s_1, s_2, \dots, s_N\rangle \mapsto |s_N, s_1, \dots, s_{N-2}\rangle$, $\hat{\boldsymbol{S}}_i \mapsto \hat{\boldsymbol{S}}_{i+1}$, is a symmetry of $\hat{H}$, $[\hat{H}, \hat{T}] = 0$. Note that $\hat{T}^N = \hat{\mathbb{1}}$, so the irreps of translation group are $R_k(\hat{T}) = e^{-\mathrm{i}\frac{2\pi}{N}k}$ for integer k (modulo N). For the $|x\rangle$ states, $\hat{T}|x\rangle = |(x+1) \mod N\rangle$.

(a) (5pts) *Show that the "ferromagnetic spin-wave" states* $|\psi_p\rangle = \sum_{x=0}^{N-1} e^{\mathrm{i}p\cdot x}|x\rangle$ *is an eigenstate of* $\hat{H}$*, where* $p = \frac{2\pi}{N}k$ *and* k *is an integer. Solve the eigenvalues as a function of* p

("the spin-wave dispersion"). [Hint: first figure out the action result of $\hat{H}$ on the $|x\rangle$ basis, then apply $\hat{H}$ on $|\psi_p\rangle$, check that the result is proportional to $|\psi_p\rangle$]

(b) (5pts) (DIFFICULT) ("Bethe ansatz") For the space with two $\uparrow$s, the basis are $|x,y\rangle \equiv \hat{S}_{x,+}\hat{S}_{y,+}|\downarrow\downarrow\dots\downarrow\rangle$ for $0 \le x < y \le (N-1)$. Consider a special case of the "Bethe ansatz", $|\psi_{p,-p}\rangle = \sum_{x,y,x<y}(e^{\mathrm{i}p\cdot x}e^{\mathrm{i}(-p)\cdot y} + e^{\mathrm{i}\theta}e^{\mathrm{i}(-p)\cdot x}e^{\mathrm{i}p\cdot y})|x,y\rangle$. *Solve the real parameters p and θ for this state to be an eigenstate of $\hat{H}$, and find the energy eigenvalue.* [Hint: apply $\hat{H}$ on this state, be careful about the "collision" case $y = x+1$; and be careful about the "boundary condition" at $x = 0$ or $y = (N-1)$, which is equivalent to the fact that $|\psi_{p,-p}\rangle$ is an eigenstate of $\hat{T}$]

Solution.

(a) Consider the action of $(\hat{\boldsymbol{S}}_i \cdot \hat{\boldsymbol{S}}_{i+1} - \frac{1}{4}) = (\hat{S}_{i,z}\hat{S}_{i+1,z} - \frac{1}{4}) + \frac{1}{2}(\hat{S}_{i,+}\hat{S}_{i+1,-} + \hat{S}_{i,-}\hat{S}_{i+1,+})$ on the $|x\rangle$ basis:

if $i \ne x$ and $(i+1) \ne x \mod N$, the result is $((-\frac{1}{2})\cdot(-\frac{1}{2}) - \frac{1}{4})|x\rangle + 0 + 0 = 0$;

if $i = x$, the result is $((\frac{1}{2})\cdot(-\frac{1}{2}) - \frac{1}{4})|x\rangle + 0 + \frac{1}{2}|x+1\rangle = \frac{1}{2}(-|x\rangle + |x+1\rangle)$;

if $i+1 = x \mod N$, the result is $((-\frac{1}{2})\cdot(\frac{1}{2}) - \frac{1}{4})|x\rangle + \frac{1}{2}|x-1\rangle + 0 = \frac{1}{2}(-|x\rangle + |x-1\rangle)$.

Therefore $\hat{H}|x\rangle = \frac{J}{2}(2|x\rangle - |x-1\rangle - |x+1\rangle)$.

Here the positions $(x-1)$, $(x+1)$ should be understood with implicit modulo N.

If we view the $\uparrow$ as a particle, $\hat{H}$ produces "hoppings" of this particle to neighboring sites.

$\hat{H}|\psi_p\rangle = \sum_{x=0}^{N-1} e^{\mathrm{i}p\cdot x}\frac{J}{2}(2|x\rangle - |(x-1) \mod N\rangle - |(x+1) \mod N\rangle)$
$= J|\psi_p\rangle - \frac{J}{2}\sum_{x'=0}^{N-1} e^{\mathrm{i}p\cdot(x'+1 \mod N)}|x'\rangle - \frac{J}{2}\sum_{x''=0}^{N-1} e^{\mathrm{i}p\cdot(x''-1 \mod N)}|x''\rangle$,
here the dummy variables $x' = (x-1) \mod N$, $x'' = (x+1) \mod N$. Because $p = \frac{2\pi}{N}k$ with integer k, $e^{\mathrm{i}p\cdot(x \mod N)} = e^{\mathrm{i}p\cdot x}$. Therefore $\hat{H}|\psi_p\rangle = (J - \frac{J}{2}e^{\mathrm{i}p} - \frac{J}{2}e^{-\mathrm{i}p})|\psi_p\rangle$.

The energy eigenvalues is $E_p = J\cdot[1-\cos(p)]$.

(b) Similar to (a), we have the following action result of $\hat{H}$ on $|x,y\rangle$ states:

if $x \ne y-1$ and $x \ne (y+1) \mod N$, $\hat{H}|x,y\rangle$
$= 2J|x,y\rangle - \frac{J}{2}(|x-1,y\rangle + |x+1,y\rangle + |x,y-1\rangle + |x,y+1\rangle)$;

if $x = y-1$, $\hat{H}|x,y\rangle = J|x,y\rangle - \frac{J}{2}(|x-1,y\rangle + |x,y+1\rangle)$;

if $x = y+1 \mod N$, $\hat{H}|x,y\rangle = J|x,y\rangle - \frac{J}{2}(|x+1,y\rangle + |x,y-1\rangle)$.

This is two "hardcore" particles' hopping (they cannot occupy the same site).

Define $\psi(x,y) = e^{\mathrm{i}px}e^{-\mathrm{i}py} + e^{\mathrm{i}\theta}e^{-\mathrm{i}px}e^{\mathrm{i}py}$ for $0 \le x < y \le N-1$, and $\psi(y,x) = \psi(x,y)$, then $|\psi_{p,-p}\rangle = \sum_{x,y,x<y} \psi(x,y)|x,y\rangle$.

For the case of $0 < x < x+1 < y < N-1$, we have

$\langle x,y|\hat{H}|\psi_{p,-p}\rangle = 2J\psi(x,y) + \frac{J}{2}[\psi(x-1,y) + \psi(x+1,y) + \psi(x,y-1) + \psi(x,y+1)]$,

plug in the formula of $\psi(x,y)$, this is

$= [2J - J\cdot(e^{-\mathrm{i}p} + e^{\mathrm{i}p})]\cdot\psi(x,y)$.

Therefore, if $|\psi_{p,-p}\rangle$ is an eigenstate of $\hat{H}$, the energy eigenvalue must be $2J\cdot[1-\cos(p)]$.

Consider the case of $0 < x < x+1 = y < N-1$,

$\langle x,x+1|\hat{H}|\psi_{p,-p}\rangle = J\psi(x,x+1) - \frac{J}{2}[\psi(x-1,x+1) + \psi(x,x+2)]$

$= J\cdot(e^{-\mathrm{i}p} + e^{\mathrm{i}\theta}e^{\mathrm{i}p}) - \frac{J}{2}\cdot(e^{-2\mathrm{i}p} + e^{\mathrm{i}\theta}e^{2\mathrm{i}p})\cdot 2$,

this should be $2J\cdot[1-\cos(p)]\cdot\psi(x,x+1) = 2J\cdot[1-\cos(p)]\cdot(e^{-\mathrm{i}p} + e^{\mathrm{i}\theta}e^{\mathrm{i}p})$.

From this we can solve $e^{\mathrm{i}\theta} = e^{-\mathrm{i}p}$. So we can choose $\theta = -p$.

Consider the case of $0 = x < x+1 < y < N-1$,

$\langle 0,y|\hat{H}|\psi_{p,-p}\rangle = 2J\psi(0,y) - \frac{J}{2}[\psi(y,N-1) + \psi(1,y) + \psi(0,y-1) + \psi(0,y+1)]$,

for this to be equal to $2J\cdot[1-\cos(p)]\cdot\psi(0,y)$

$= 2J\psi(0,y) - \frac{J}{2}[\psi(-1,y) + \psi(1,y) + \psi(0,y-1) + \psi(0,y+1)]$,

we must have $\psi(y,N-1) = e^{\mathrm{i}py}e^{-\mathrm{i}p(N-1)} + e^{\mathrm{i}\theta}e^{-\mathrm{i}py}e^{\mathrm{i}p(N-1)}$

$= \psi(-1,y) = e^{-\mathrm{i}p}e^{-\mathrm{i}py} + e^{\mathrm{i}\theta}e^{\mathrm{i}p}e^{\mathrm{i}py}$, for all $1 < y < N-1$.

Therefore $e^{\mathrm{i}\theta}e^{\mathrm{i}pN} = 1$, together with $\theta = -p$ we have $e^{\mathrm{i}p(N-1)} = 1$.

Finally,

$E_{p,-p} = 2J\cdot[1-\cos(p)]$,

$\theta = -p$,

$p = \frac{2\pi}{N-1}k$ with integer k.

Note: as a check, consider $N = 4$ case:

$-\frac{E_p}{J} + 1 = \cos(\frac{2\pi}{4}k) = 1$ or 0 or -1, and

$-\frac{E_{p,-p}}{J} + 1 = 2\cos(\frac{2\pi}{3}k) - 1 = 1$ or -2.

These are some of the eigenvalues in problem 3(c).