Advanced Quantum Mechanics: Fall 2018
Final Exam: Brief Solutions

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

Possibly Useful facts:

- $\epsilon_{abc} \equiv \begin{cases} +1, & abc = xyz, \text{ or } yzx, \text{ or } zxy; \\ -1, & abc = zyx, \text{ or } xzy, \text{ or } yxz; \\ 0, & \text{otherwise.} \end{cases}$ $\epsilon_{abc} = \epsilon_{bca} = -\epsilon_{acb}$. $\delta_{ab} \equiv \begin{cases} 1, & a = b; \\ 0, & a \neq b. \end{cases}$
- Some Taylor expansions: $\exp(x) = \sum_{n=0}^{\infty} \frac{x^n}{n!} = 1 + x + \frac{x^2}{2} + \frac{x^3}{6} + O(x^4)$, $\sqrt{1+x} = 1 + \frac{1}{2}x - \frac{1}{8}x^2 + \frac{1}{16}x^3 + O(x^4)$, $\frac{1}{\sqrt{1+x}} = 1 - \frac{1}{2}x + \frac{3}{8}x^2 - \frac{5}{16}x^3 + O(x^4)$.
- 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 $[\hat{S}_a, \hat{S}_b] = \mathbb{i} \sum_c \epsilon_{abc} \hat{S}_c$. $(a, b, c = x, y, z)$
  - $\hat{\boldsymbol{S}}^2 \equiv \sum_a \hat{S}_a^2$ commutes with $\hat{S}_{x,y,z}$. Basis $|S, m\rangle$ satisfy, $\hat{S}_z |S, m\rangle = m|S, m\rangle$, $\hat{\boldsymbol{S}}^2 |S, m\rangle = S(S + 1)|S, m\rangle$. $2S$ is non-negative integer, $m = -S, -S + 1, \ldots, S$.
  - 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 $\hat{S}_\pm |S, S_z = m\rangle = \sqrt{(S \mp m)(S \pm m + 1)} |S, S_z = m \pm 1\rangle$.
  - $e^{-\mathbb{i}\theta \boldsymbol{n}\cdot\hat{\boldsymbol{S}}} \cdot \hat{S}_a \cdot e^{\mathbb{i}\theta \boldsymbol{n}\cdot\hat{\boldsymbol{S}}} = \sum_b \hat{S}_b \cdot [R_{\boldsymbol{n}}(\theta)]_{ba}$. $SO(3)$ matrix for rotation around axis $\boldsymbol{n}$ by angle θ is $[R_{\boldsymbol{n}}(\theta)]_{ab} = n_a n_b + \cos\theta(\delta_{ab} - n_a n_b) - \sin\theta \sum_c \epsilon_{abc} n_c$, here $\boldsymbol{n}$ is 3D unit-length real vector, $\boldsymbol{n} \cdot \hat{\boldsymbol{S}} \equiv n_x \hat{S}_x + n_y \hat{S}_y + n_z \hat{S}_z$.
  - $\hat{\boldsymbol{S}}_i \cdot \hat{\boldsymbol{S}}_j \equiv \hat{S}_{iz}\hat{S}_{jz} + \hat{S}_{ix}\hat{S}_{jx} + \hat{S}_{iy}\hat{S}_{jy} = \hat{S}_{iz}\hat{S}_{jz} + \frac{1}{2}(\hat{S}_{i+}\hat{S}_{j-} + \hat{S}_{i-}\hat{S}_{j+})$.
- Spin-1/2: $\hat{S}_a = \sigma_a/2$ under the $\hat{S}_z$ eigenbasis $(a = x, y, z)$.
  Pauli matrices σ_a are $\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$, $\sigma_y = \begin{pmatrix} 0 & -\mathbb{i} \\ \mathbb{i} & 0 \end{pmatrix}$, $\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$. $\{\sigma_a, \sigma_b\} = 2\delta_{ab}\mathbb{1}$.
  $\exp(-\mathbb{i}\theta \boldsymbol{n} \cdot \boldsymbol{\sigma}) = \cos(\theta)\mathbb{1} - \mathbb{i}\sin(\theta)(\boldsymbol{n} \cdot \boldsymbol{\sigma})$. $|\hat{S}_z = \pm\frac{1}{2}\rangle$ are denoted by $|\uparrow\rangle$ and $|\downarrow\rangle$.
- 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_3 group: $\{(C_3)^{(n \mod 3)}(\sigma)^{(m \mod 2)} | C_3^3 = \sigma^2 = C_3\sigma C_3\sigma = \mathbb{1}\}$.
  6 elements, 3 conjugacy classes, $\{\mathbb{1}\}$, $\{C_3, C_3^2\}$, and $\{\sigma, C_3\sigma, C_3^2\sigma\}$.
  Character table χ_{Γ_i} for irreducible representations (irrep) $\Gamma_{1,2,3}$ is given on the right.

	$\mathbb{1}$	$2C_3$	3σ
Γ_1	1	1	1
Γ_2	1	1	-1
Γ_3	2	-1	0

Problem 1. (30 points) Consider two spin-1 moments, $\hat{\boldsymbol{S}}_1$ and $\hat{\boldsymbol{S}}_2$. They satisfy $[\hat{S}_{i,a}, \hat{S}_{j,b}] = \delta_{i,j} \sum_c \mathbb{i}\epsilon_{abc}\hat{S}_{i,c}$ (here a, b, c label x, y, z components), $\hat{\boldsymbol{S}}_1^2 = \hat{\boldsymbol{S}}_2^2 = 1 \cdot (1+1) = 2$. A complete orthonormal basis for the 9-dimensional Hilbert space is the $\hat{S}_z$-basis, $|S_{1,z}\rangle|S_{2,z}\rangle$. Here $S_{i,z} = 1, 0, -1$ 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 $a = x, y, z$ under S_z-basis are given on page 1.

(a) (10pts) *Write down all 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) (3pts) Define $\hat{\chi}_z = \hat{S}_{1,x}\hat{S}_{2,y} - \hat{S}_{1,y}\hat{S}_{2,x}$. *Show by explicit calculation that* $[\hat{\chi}_z, \hat{S}_z] = 0$. Here $\hat{S}_z \equiv \hat{S}_{1,z} + \hat{S}_{2,z}$.

(c) (5pts) *Compute* $\exp[-\mathbb{i}\theta \cdot (\hat{S}_{1,z} - \hat{S}_{2,z})] \cdot \hat{\chi}_z \cdot \exp[\mathbb{i}\theta \cdot (\hat{S}_{1,z} - \hat{S}_{2,z})]$. *$\theta$ is a real number. The result should be a finite-degree polynomial of spin operators.* [Hint: check page 1]

(d) (7pts) The full Hamiltonian is $\hat{H} = \hat{H}_0 + D\hat{\chi}_z$. D is a real "small" parameter. *Solve the perturbed energy eigenvalue(s) of $\hat{H}$ corresponding to the original ground state(s) to second order of D.* [Hint: the original ground states of $\hat{H}_0$ are degenerate, but you can avoid degenerate perturbation theory by dividing Hilbert space by symmetry; some previous results might help]

(e) (5pts**) Denote the ground states of $\hat{H}_0$ in (a) by $|\psi_{0,\alpha}^{(0)}\rangle$ where α labels degenerate states. Let $|\psi(t=0)\rangle = |S_{1,z} = +1\rangle|S_{2,z} = -1\rangle$, and $|\psi(t)\rangle = e^{-\mathbb{i}\hat{H}\cdot t/\hbar}|\psi(t=0)\rangle$. *Compute the "ground state probability"* $P_0(|\psi(t)\rangle) = \sum_\alpha |\langle\psi_{0,\alpha}^{(0)}|\psi(t)\rangle|^2$ *by time-dependent perturbation theory to second order of D.* [Hint: $|\psi(t=0)\rangle$ is NOT $\hat{H}_0$ eigenstate, but interaction picture can still be used, $|\langle\psi_{0,\alpha}^{(0)}|\psi(t)\rangle|^2 = |\langle\psi_{0,\alpha}^{(0)}|\hat{U}_I(t)|\psi(t=0)\rangle|^2$, where $\hat{U}_I(t) = e^{\mathbb{i}\hat{H}_0\cdot t/\hbar}e^{-\mathbb{i}\hat{H}\cdot t/\hbar}$; due to some symmetry, you do not need to compute $\langle\psi_{0,\alpha}^{(0)}|\psi(t)\rangle$ for every α]

Solution

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

$\hat{H}_0 = -\frac{J}{2}(\hat{\boldsymbol{S}}_1 + \hat{\boldsymbol{S}}_2)^2 + 2J$.

The total spin quantum number can be 2 or 1 or 0, "$\mathbf{1} \otimes \mathbf{1} = \mathbf{2} \oplus \mathbf{1} \oplus \mathbf{0}$".

The basis states $|S_{1+2}, S_{1+2,z}\rangle$ are eigenstates of $\hat{H}_0$, and can be built in similar way as that of Homework #5 Problem 3(a,b). First solve the highest S_z state in each total S_{1+2} subspace, then the other states can be obtained by applications of lowering ladder operators.

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

$\hat{H}_0$ eigenvalue	S_{1+2}	$S_{1+2,z}$	state
$-J$	2	2	$\|1\rangle\|1\rangle$
$-J$	2	1	$\frac{1}{\sqrt{2}}(\|1\rangle\|0\rangle + \|0\rangle\|1\rangle)$
$-J$	2	0	$\frac{1}{\sqrt{6}}(\|1\rangle\|-1\rangle + 2\|0\rangle\|0\rangle + \|-1\rangle\|1\rangle)$
$-J$	2	-1	$\frac{1}{\sqrt{2}}(\|0\rangle\|-1\rangle + \|-1\rangle\|0\rangle)$
$-J$	2	-2	$\|-1\rangle\|-1\rangle$
J	1	1	$\frac{1}{\sqrt{2}}(\|1\rangle\|0\rangle - \|0\rangle\|1\rangle)$
J	1	0	$\frac{1}{\sqrt{2}}(\|1\rangle\|-1\rangle - \|-1\rangle\|1\rangle)$
J	1	-1	$\frac{1}{\sqrt{2}}(\|0\rangle\|-1\rangle - \|-1\rangle\|0\rangle)$
$2J$	0	0	$\frac{1}{\sqrt{3}}(\|1\rangle\|-1\rangle - \|0\rangle\|0\rangle + \|-1\rangle\|1\rangle)$

(b) This is part of Homework #6 Problem 1(2).

$[\hat{S}_{1,z} + \hat{S}_{2,z}, \hat{S}_{1,x}\hat{S}_{2,y} - \hat{S}_{1,y}\hat{S}_{2,x}] = \mathbb{i}\hat{S}_{1,y}\hat{S}_{2,y} - (-\mathbb{i}\hat{S}_{1,x})\hat{S}_{2,x} + \hat{S}_{1,x}(-\mathbb{i}\hat{S}_{2,x}) - \hat{S}_{1,y}(\mathbb{i}\hat{S}_{2,y}) = 0$.

This can also be proved by $\hat{\chi}_z = \frac{1}{2}(\mathbb{i}\hat{S}_{1,+}\hat{S}_{2,-} - \mathbb{i}\hat{S}_{1,-}\hat{S}_{2,+})$, and $[\hat{S}_{1,z} + \hat{S}_{2,z}, \hat{S}_{i,\pm}] = \pm\hat{S}_{i,\pm}$.

(c) Method #1: use the results on page 1,

$e^{-\mathbb{i}\theta\hat{S}_z}\hat{S}_x e^{\mathbb{i}\theta\hat{S}_z} = \hat{S}_x\cos\theta + \hat{S}_y\sin\theta$, $e^{-\mathbb{i}\theta\hat{S}_z}\hat{S}_y e^{\mathbb{i}\theta\hat{S}_z} = \hat{S}_y\cos\theta - \hat{S}_x\sin\theta$.

Then $\exp[-\mathbb{i}\theta\cdot(\hat{S}_{1,z} - \hat{S}_{2,z})]\cdot\hat{\chi}_z\cdot\exp[\mathbb{i}\theta\cdot(\hat{S}_{1,z} - \hat{S}_{2,z})]$

$= (\hat{S}_{1,x}\cos\theta + \hat{S}_{1,y}\sin\theta)(\hat{S}_{2,y}\cos\theta + \hat{S}_{2,x}\sin\theta) - (\hat{S}_{1,y}\cos\theta - \hat{S}_{1,x}\sin\theta)(\hat{S}_{2,x}\cos\theta - \hat{S}_{2,y}\sin\theta)$

$= \cos(2\theta)\hat{\chi}_z + \sin(2\theta)(\hat{S}_{1,x}\hat{S}_{2,x} + \hat{S}_{1,y}\hat{S}_{2,y})$.

Method #2: directly use Baker-Hausdorff formula,

let $\hat{A} = -\frac{1}{2}\mathbb{i}(\hat{S}_{1,z} - \hat{S}_{2,z})$, $\hat{B} = \hat{\chi}_z$, $\hat{C} = (\hat{S}_{1,x}\hat{S}_{2,x} + \hat{S}_{1,y}\hat{S}_{2,y})$, then $[\hat{A}, \hat{B}] = \hat{C}$, $[\hat{A}, \hat{C}] = -\hat{B}$.

use the result of Homework #1 Problem 5, $\exp[-\mathbb{i}\theta \cdot (\hat{S}_{1,z} - \hat{S}_{2,z})] \cdot \hat{\chi}_z \cdot \exp[\mathbb{i}\theta \cdot (\hat{S}_{1,z} - \hat{S}_{2,z})]$

$= \exp(2\theta\hat{A})\hat{B}\exp(-2\theta\hat{A}) = \hat{B}\cos(2\theta) + \hat{C}\sin(2\theta)$

$= \cos(2\theta)\hat{\chi}_z + \sin(2\theta)(\hat{S}_{1,x}\hat{S}_{2,x} + \hat{S}_{1,y}\hat{S}_{2,y})$.

(d) This is similar to Homework #6 Problem 1(3)

Method #1: divide Hilbert space by symmetry, then use perturbation theory,

$\hat{H}$ conserves total $\hat{S}_{1+2,z} \equiv \hat{S}_{1,z} + \hat{S}_{2,z}$, $[\hat{H}, \hat{S}_z] = 0$. Therefore $\hat{H}$ is block-diagonalized by dividing the 9-dimensional Hilbert space into different total-S_z subspaces.

The $S_{1+2,z} = \pm 2$ subspaces are 1-dimensional with the complete orthonormal basis $(|S_{1+2} = 2, S_{1+2,z} = \pm 2\rangle)$.

The $S_{1+2,z} = \pm 1$ subspaces are 2-dimensional with the complete orthonormal basis $(|S_{1+2} = 2, S_{1+2,z} = \pm 1\rangle, |S_{1+2} = 1, S_{1+2,z} = \pm 1\rangle)$.

The $S_{1+2,z} = 0$ subspace is 3-dimensional with the complete orthonormal basis $(|S_{1+2} = 2, S_{1+2,z} = 0\rangle, |S_{1+2} = 1, S_{1+2,z} = 0\rangle, |S_{1+2} = 0, S_{1+2,z} = 0\rangle)$.

In each subspace, the ground state of $\hat{H}_0$ is non-degenerate, $|S_{1+2} = 2, S_{1+2,z}\rangle$, so one can use non-degenerate perturbation theory.

To compute the matrix elements of the perturbation, it may be more convenient to use $\hat{\chi}_z = \frac{1}{2}(\mathbb{i}\hat{S}_{1,+}\hat{S}_{2,-} - \mathbb{i}\hat{S}_{1,-}\hat{S}_{2,+})$, and $\hat{S}_{i,+}|S_{i,z} = 0\rangle = \sqrt{2}|S_{i,z} = 1\rangle$, ...

$S_{1+2,z}$	$\hat{H}$ in subspace	2nd order ground state energy
2	$(-J) + (0)$	$-J$
1	$\begin{pmatrix} -J & 0 \\ 0 & J \end{pmatrix} + \begin{pmatrix} 0 & -\mathbb{i}D \\ \mathbb{i}D & 0 \end{pmatrix}$	$\approx -J + \frac{(-\mathbb{i}D)\cdot(\mathbb{i}D)}{-J-J} = -J - \frac{D^2}{2J}$
0	$\begin{pmatrix} -J & 0 & 0 \\ 0 & J & 0 \\ 0 & 0 & 2J \end{pmatrix} + \begin{pmatrix} 0 & -\frac{2\mathbb{i}}{\sqrt{3}}D & 0 \\ \frac{2\mathbb{i}}{\sqrt{3}}D & 0 & -\sqrt{\frac{2}{3}}\mathbb{i}D \\ 0 & \sqrt{\frac{2}{3}}\mathbb{i}D & 0 \end{pmatrix}$	$\approx -J + \frac{(-2\mathbb{i}D/\sqrt{3})\cdot(2\mathbb{i}D/\sqrt{3})}{-J-J} = -J - \frac{2D^2}{3J}$
-1	$\begin{pmatrix} -J & 0 \\ 0 & J \end{pmatrix} + \begin{pmatrix} 0 & -\mathbb{i}D \\ \mathbb{i}D & 0 \end{pmatrix}$	$\approx -J + \frac{(-\mathbb{i}D)\cdot(\mathbb{i}D)}{-J-J} = -J - \frac{D^2}{2J}$
-2	$(-J) + (0)$	$-J$

Method #2: compute the exact eigenvalues of $\hat{H}$ using the result of 1(c),

$\hat{H} = -J\hat{S}_{1,z}\hat{S}_{2,z} - J(\hat{S}_{1,x}\hat{S}_{2,x} + \hat{S}_{1,y}\hat{S}_{2,y}) + D\hat{\chi}_z$.

By applying unitary $\hat{U} = e^{-\mathbb{i}\theta(\hat{S}_{1,z}-\hat{S}_{2,z})}$ with appropriate θ, we can get $\hat{U}\hat{H}\hat{U}^\dagger$ $= -J\hat{S}_{1,z}\hat{S}_{2,z} - \sqrt{J^2+D^2}(\hat{S}_{1,x}\hat{S}_{2,x} + \hat{S}_{1,y}\hat{S}_{2,y}) = -\sqrt{J^2+D^2}\boldsymbol{\hat{J}}_1\cdot\boldsymbol{\hat{J}}_2 + (\sqrt{J^2+D^2}-J)\hat{S}_{1,z}\hat{S}_{2,z}$. Here $(\cos\theta, \sin\theta) = (\frac{J}{\sqrt{J^2+D^2}}, -\frac{D}{\sqrt{J^2+D^2}})$. $\hat{U}\hat{H}\hat{U}^\dagger$ and $\hat{H}$ have the same eigenvalues.

$\hat{U}\hat{H}\hat{U}^\dagger$ still conserves total $\hat{S}_z$. Use the basis in Method #1.

In $S_z = \pm 2$ subspace, $\hat{U}\hat{H}\hat{U}^\dagger$ is the 1×1 matrix, $(-\sqrt{J^2+D^2}) + (\sqrt{J^2+D^2}-J) = (-J)$, with ground state eigenvalues $-J$.

In $S_z = \pm 1$ subspace, $\hat{U}\hat{H}\hat{U}^\dagger$ is the 2×2 diagonal matrix, $\begin{pmatrix} -\sqrt{J^2+D^2} & 0 \\ 0 & \sqrt{J^2+D^2} \end{pmatrix}$, with ground state eigenvalue $-\sqrt{J^2+D^2} \approx -J - \frac{D^2}{2J} + O(D^4)$.

In $S_z = 0$ subspace, $\hat{U}\hat{H}\hat{U}^\dagger$ is a 3×3 matrix, $\sqrt{J^2+D^2}\cdot \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 2 \end{pmatrix}$ $+(\sqrt{J^2+D^2} - J)\cdot \begin{pmatrix} -\frac{1}{3} & 0 & -\frac{\sqrt{2}}{3} \\ 0 & -1 & 0 \\ -\frac{\sqrt{2}}{3} & 0 & -\frac{2}{3} \end{pmatrix}$. We only need to solve a 2×2 problem, $\frac{J}{2}\sigma_0 - \frac{\sqrt{2}}{3}(\sqrt{J^2+D^2}-J)\sigma_1 - (\frac{4}{3}\sqrt{J^2+D^2}+\frac{J}{6})\sigma_3$, for the first and last basis. The ground state eigenvalue is $\frac{J}{2} - \sqrt{\frac{2}{9}(\sqrt{J^2+D^2}-J)^2 + (\frac{4}{3}\sqrt{J^2+D^2}+\frac{J}{6})^2} \approx \frac{J}{2} - \frac{3}{2}\sqrt{(J+\frac{4D^2}{9J})^2 + O(D^4)}$ $\approx \frac{J}{2} - \frac{3}{2}(J + \frac{4D^2}{9J}) + O(D^4) \approx -J - \frac{2D^2}{3J} + O(D^4)$.

(e) Use interaction picture. Define interaction picture operator for the perturbation, $\hat{V}_I(t) \equiv e^{\mathbb{i}\hat{H}_0\cdot t/\hbar}\cdot(D\hat{\chi}_z)\cdot e^{-\mathbb{i}\hat{H}_0\cdot t/\hbar}$. Then the interaction picture time evolution operator is $\hat{U}_I(t) \equiv e^{\mathbb{i}\hat{H}_0\cdot t/\hbar}e^{-\mathbb{i}\hat{H}\cdot t/\hbar} = \mathbb{1} + \frac{-\mathbb{i}}{\hbar}\int_0^t \mathrm{d}t_1\,\hat{V}_I(t_1) + (\frac{-\mathbb{i}}{\hbar})^2\int_0^t \mathrm{d}t_1\int_0^{t_1}\mathrm{d}t_2\,\hat{V}_I(t_1)\hat{V}_I(t_2) + \ldots$

The original ground states are $|S_{1+2}=2, S_{1+2,z}\rangle$ for $S_{1+2,z} = -2,-1,0,1,2$. Note that $\hat{V}_I(t)$ still conserves total $\hat{S}_z$. So only $\langle S_{1+2}=2, S_{1+2,z}=0|\hat{U}_I|\psi(t=0)\rangle$ is nonzero.

In the $S_z = 0$ subspace with the three basis given in (d),

$\hat{V}_I(t)$ is $\begin{pmatrix} 0 & -\frac{2\mathbb{i}}{\sqrt{3}}D\cdot e^{-\mathbb{i}2J/\hbar\cdot t} & 0 \\ \frac{2\mathbb{i}}{\sqrt{3}}D\cdot e^{\mathbb{i}2J/\hbar\cdot t} & 0 & -\sqrt{\frac{2}{3}}\mathbb{i}D\cdot e^{-\mathbb{i}J/\hbar\cdot t} \\ 0 & \sqrt{\frac{2}{3}}\mathbb{i}D\cdot e^{\mathbb{i}J/\hbar\cdot t} & 0 \end{pmatrix}$, $|\psi(t=0)\rangle$ is $\begin{pmatrix} \frac{1}{\sqrt{6}} \\ \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{3}} \end{pmatrix}$. Then

$\langle S_{1+2}=2, S_{1+2,z}=0|\hat{U}_I|\psi(t=0)\rangle \approx \frac{1}{\sqrt{6}} + \frac{-\mathbb{i}}{\hbar}\int_0^t \mathrm{d}t_1\,[-\frac{2\mathbb{i}}{\sqrt{3}}D\cdot e^{-\mathbb{i}2J/\hbar\cdot t_1}\cdot\frac{1}{\sqrt{2}}]$

$+(\frac{-\mathbb{i}}{\hbar})^2\int_0^t \mathrm{d}t_1\int_0^{t_1}\mathrm{d}t_2\,[\frac{-2\mathbb{i}}{\sqrt{3}}De^{-\mathbb{i}2J/\hbar\cdot t_1}][\frac{2\mathbb{i}}{\sqrt{3}}De^{\mathbb{i}2J/\hbar\cdot t_2}\cdot\frac{1}{\sqrt{6}} + \frac{-\sqrt{2}\mathbb{i}}{\sqrt{3}}De^{-\mathbb{i}J/\hbar\cdot t_2}\cdot\frac{1}{\sqrt{3}}] + \ldots$

$\approx \frac{1}{\sqrt{6}} - \frac{\mathbb{i}D}{\sqrt{6}J}(e^{-\mathbb{i}2Jt/\hbar}-1) + \frac{-\mathbb{i}}{\hbar}\int_0^t \mathrm{d}t_1\,[\frac{-2\mathbb{i}}{\sqrt{3}}De^{-\mathbb{i}2J/\hbar\cdot t_1}][\frac{-\mathbb{i}D}{3\sqrt{2}J}(e^{\mathbb{i}2Jt_1/\hbar}-1) + \frac{-\mathbb{i}\sqrt{2}D}{3J}(e^{-\mathbb{i}Jt_1/\hbar}-1)]$

$\approx \frac{1}{\sqrt{6}} - \frac{\mathbb{i}D}{\sqrt{6}J}(e^{-\mathbb{i}2Jt/\hbar}-1) + \frac{-\mathbb{i}}{\hbar}\int_0^t \mathrm{d}t_1\,[\frac{-2\mathbb{i}}{\sqrt{3}}De^{-\mathbb{i}2J/\hbar\cdot t_1}][\frac{-\mathbb{i}D}{3\sqrt{2}J}e^{\mathbb{i}2Jt_1/\hbar} + \frac{\mathbb{i}\sqrt{2}D}{2J} + \frac{-\mathbb{i}\sqrt{2}D}{3J}e^{-\mathbb{i}Jt_1/\hbar}]$

$\approx \frac{1}{\sqrt{6}} - \frac{\mathrm{i}D}{\sqrt{6}J}(e^{-\mathrm{i}2Jt/\hbar} - 1) + \frac{\mathrm{i}2D^2}{3\sqrt{6}\hbar J}t + \frac{\sqrt{2}D^2}{2\sqrt{3}J^2}(e^{-\mathrm{i}2Jt/\hbar} - 1) - \frac{2\sqrt{2}D^2}{9\sqrt{3}J^2}(e^{-\mathrm{i}3Jt/\hbar} - 1).$

Take the square of absolute value of the above result of $\langle S_{1+2} = 2, S_{1+2,z} = 0|\hat{U}_I|\psi(t=0)\rangle$, keep up to D^2 order, because the imaginary part of $\langle S_{1+2} = 2, S_{1+2,z} = 0|\hat{U}_I|\psi(t=0)\rangle$ has no $O(1)$ term, we only need to keep $O(D)$ term in the imaginary part of this amplitude,

$P_0(|\psi(t)\rangle)$

$\approx [\frac{1}{\sqrt{6}} - \frac{D}{\sqrt{6}J}\sin(\frac{2Jt}{\hbar}) + \frac{\sqrt{2}D^2}{2\sqrt{3}J^2}(\cos(\frac{2Jt}{\hbar}) - 1) - \frac{2\sqrt{2}D^2}{9\sqrt{3}J^2}(\cos(\frac{3Jt}{\hbar}) - 1)]^2 + [\frac{D}{\sqrt{6}J}(\cos(\frac{2Jt}{\hbar}) - 1)]^2$

$\approx \frac{1}{6} - \frac{D}{3J}\sin(\frac{2Jt}{\hbar}) + \frac{D^2}{J^2}[\frac{1}{6}\sin^2(\frac{2Jt}{\hbar}) + \frac{1}{3}(\cos(\frac{2Jt}{\hbar}) - 1) - \frac{4}{27}(\cos(\frac{3Jt}{\hbar}) - 1) + \frac{1}{6}(\cos(\frac{2Jt}{\hbar}) - 1)^2]$

$\approx \frac{1}{6} - \frac{D}{3J}\sin(\frac{2Jt}{\hbar}) - \frac{4D^2}{27J^2}(\cos(\frac{3Jt}{\hbar}) - 1)$.

Some consistency check:

when $t = 0$ this should be $|\langle S_{1+2} = 2, S_{1+2,z} = 0|\psi(t=0)\rangle|^2 = \frac{1}{6}$;

this should be an oscillating function, has no terms $\propto t$ or $\propto t^2$ (because there is no "resonance', namely time-independent perturbation connecting degenerate levels).

Problem 2 (35 points) Consider three spin-1/2 moments, labeled by $i = 1, 2, 3$. The spin operators satisfy $[\hat{S}_{i,a}, \hat{S}_{j,b}] = \delta_{ij}\sum_c \mathrm{i}\epsilon_{abc}\hat{S}_{i,c}$ for $i, j = 1, 2, 3$ and $a, b, c = x, y, z$, and $(\hat{\boldsymbol{S}}_i)^2 = \frac{1}{2}\cdot(\frac{1}{2}+1) = \frac{3}{4}$. A complete orthonormal basis $|\psi_i\rangle$ $(i = 1, \ldots, 8)$ is the S_z-basis, $|S_{1z}, S_{2z}, S_{3z}\rangle$, namely $|\uparrow\uparrow\uparrow\rangle$, $|\downarrow\uparrow\uparrow\rangle$, $|\uparrow\downarrow\uparrow\rangle$, $|\uparrow\uparrow\downarrow\rangle$, $|\uparrow\downarrow\downarrow\rangle$, $|\downarrow\uparrow\downarrow\rangle$, $|\downarrow\downarrow\uparrow\rangle$, $|\downarrow\downarrow\downarrow\rangle$.

(a) (10pts) Consider the D_3 discrete symmetry (see page 1) generated by

$C_3: \ \hat{\boldsymbol{S}}_1 \mapsto \hat{\boldsymbol{S}}_2, \ \hat{\boldsymbol{S}}_2 \mapsto \hat{\boldsymbol{S}}_3, \ \hat{\boldsymbol{S}}_3 \mapsto \hat{\boldsymbol{S}}_1$; and $\sigma: \ \hat{\boldsymbol{S}}_1 \mapsto \hat{\boldsymbol{S}}_1, \ \hat{\boldsymbol{S}}_2 \mapsto \hat{\boldsymbol{S}}_3, \ \hat{\boldsymbol{S}}_3 \mapsto \hat{\boldsymbol{S}}_2$.

Their actions on S_z-basis are $\hat{C}_3|s_1, s_2, s_3\rangle = |s_3, s_1, s_2\rangle$, and $\hat{\sigma}|s_1, s_2, s_3\rangle = |s_1, s_3, s_2\rangle$. Note that D_3 group actions do not change total $\hat{S}_z = \sum_{i=1}^3 \hat{S}_{i,z}$. Therefore the 8×8 matrices, $\langle\psi_i|\hat{C}_3|\psi_j\rangle$ and $\langle\psi_i|\hat{\sigma}|\psi_j\rangle$, are block-diagonal within each total-S_z subspace. *Write down the diagonal blocks of* $\langle\psi_i|\hat{C}_3|\psi_j\rangle$ *and* $\langle\psi_i|\hat{\sigma}|\psi_j\rangle$, *namely representation matrices,* $R_{\hat{S}_z=m}(C_3)$ *and* $R_{\hat{S}_z=m}(\sigma)$, *for each total-*S_z *subspace (for* $S_z = \frac{3}{2}, \frac{1}{2}, -\frac{1}{2}, -\frac{3}{2}$, *respectively).*

(b) (10pts*) Some of the representations in (a) are reducible. Make orthonormal linear combinations of the S_z-basis, so that they are eigenstates of $\hat{S}_z$ and form irreducible representations of the D_3 group. *Copy the following table to your answer sheet and fill the complete orthonormal irreducible representation basis states (in terms of* S_z*-basis) into the last row.* [NOTE: some entries will be empty; the ladder operators $\hat{S}_\pm = \sum_{i=1}^3 \hat{S}_{i,\pm}$ are invariant under D_3 group, so if you find a state $|\hat{S}_z = m, \Gamma_i\rangle$, then you can generate $|\hat{S}_z = m\pm 1, \Gamma_i\rangle \propto \hat{S}_\pm|\hat{S}_z = m, \Gamma_i\rangle$; note that Γ_3 is 2-dimensional irrep; you can use the "projection operator" $\sum_{g\in D_3}[\chi_{\Gamma_i}(g)]^* \cdot \hat{g}|\psi_j\rangle$ to generate these irrep basis, remember to orthonormalize the results]

$\sum_{i=1}^3 \hat{S}_{i,z}$	$\frac{3}{2}$			$\frac{1}{2}$			$-\frac{1}{2}$			$-\frac{3}{2}$		
D_3 irrep.	Γ_1	Γ_2	Γ_3	Γ_1	Γ_2	Γ_3	Γ_1	Γ_2	Γ_3	Γ_1	Γ_2	Γ_3
basis state(s)												

(c) (10pts) Consider $\hat{H} = (\hat{S}_{1,x}\hat{S}_{2,x} + \hat{S}_{1,y}\hat{S}_{2,y}) + (\hat{S}_{2,x}\hat{S}_{3,x} + \hat{S}_{2,y}\hat{S}_{3,y}) + (\hat{S}_{3,x}\hat{S}_{1,x} + \hat{S}_{3,y}\hat{S}_{1,y})$ $= \frac{1}{2}(\hat{S}_{1,+}\hat{S}_{2,-} + \hat{S}_{1,-}\hat{S}_{2,+}) + \frac{1}{2}(\hat{S}_{2,+}\hat{S}_{3,-} + \hat{S}_{2,-}\hat{S}_{3,+}) + \frac{1}{2}(\hat{S}_{3,+}\hat{S}_{1,-} + \hat{S}_{3,-}\hat{S}_{1,+})$. It is easy to see that $[\hat{H}, \sum_{i=1}^3 \hat{S}_{i,z}] = 0$, and $\hat{H}$ is invariant under D_3 group. *Solve the eigenvalues and eigenstates(in terms of S_z tensor product basis) for $\hat{H}$.* [Hint: results of (b) may help, also consider the difference between $\hat{H}$ and $\hat{\boldsymbol{S}}_1\cdot\hat{\boldsymbol{S}}_2+\hat{\boldsymbol{S}}_2\cdot\hat{\boldsymbol{S}}_3+\hat{\boldsymbol{S}}_3\cdot\hat{\boldsymbol{S}}_1 = \frac{1}{2}(\hat{\boldsymbol{S}}_1+\hat{\boldsymbol{S}}_2+\hat{\boldsymbol{S}}_3)^2$+constant]

(d) (5pts) *Explain the reason why the eigenvalues in (c) have degeneracy.*

Solution

(a) Under the S_z basis given in the problem.

For $S_z = \pm\frac{3}{2}$ subspace, $R_{\hat{S}_z=\pm\frac{3}{2}}(C_3) = (1)$, $R_{\hat{S}_z=\pm\frac{3}{2}}(\sigma) = (1)$.

For $\S_z = \pm\frac{1}{2}$ subspace, $R_{\hat{S}_z=\pm\frac{1}{2}}(C_3) = \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}$, $R_{\hat{S}_z=\pm\frac{1}{2}}(\sigma) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}$.

(b) This is exactly the same as Homework #5 Problem 4(c).

Note that $\hat{\boldsymbol{S}}^2 \equiv (\sum_{i=1}^3 \hat{\boldsymbol{S}}_i)^2$ is invariant under D_3 group. So we can also label these states by the total spin quantum number.

The choice of basis for Γ_3 representation is not unique.

$\sum_{i=1}^3 \hat{S}_{i,z}$	$\frac{3}{2}$	$\frac{1}{2}$	
D_3 irrep	Γ_1	Γ_1	Γ_3
total spin $\sum_{i=1}^3 \hat{\boldsymbol{S}}_i$	$\frac{3}{2}$	$\frac{3}{2}$	$\frac{1}{2}$
basis state(s)	$\lvert\uparrow\uparrow\uparrow\rangle$	$\frac{1}{\sqrt{3}}(\lvert\downarrow\uparrow\uparrow\rangle + \lvert\uparrow\downarrow\uparrow\rangle + \lvert\uparrow\uparrow\downarrow\rangle)$	$\begin{cases} \frac{1}{\sqrt{6}}(2\lvert\downarrow\uparrow\uparrow\rangle - \lvert\uparrow\downarrow\uparrow\rangle - \lvert\uparrow\uparrow\downarrow\rangle) \\ \frac{1}{\sqrt{2}}(\lvert\uparrow\downarrow\uparrow\rangle - \lvert\uparrow\uparrow\downarrow\rangle) \end{cases}$

$\sum_{i=1}^3 \hat{S}_{i,z}$	$-\frac{1}{2}$		$-\frac{3}{2}$
D_3 irrep	Γ_1	Γ_3	Γ_1
total spin $\sum_{i=1}^3 \hat{\boldsymbol{S}}_i$	$\frac{3}{2}$	$\frac{1}{2}$	$\frac{3}{2}$
basis state(s)	$\frac{1}{\sqrt{3}}(\lvert\uparrow\downarrow\downarrow\rangle + \lvert\downarrow\uparrow\downarrow\rangle + \lvert\downarrow\downarrow\uparrow\rangle)$	$\begin{cases} \frac{1}{\sqrt{6}}(2\lvert\uparrow\downarrow\downarrow\rangle - \lvert\downarrow\uparrow\downarrow\rangle - \lvert\downarrow\downarrow\uparrow\rangle) \\ \frac{1}{\sqrt{2}}(\lvert\downarrow\uparrow\downarrow\rangle - \lvert\downarrow\downarrow\uparrow\rangle) \end{cases}$	$\lvert\downarrow\downarrow\downarrow\rangle$

(c) Method #1:

$\hat{H} = \frac{1}{2}\left[(\hat{S}_{1,x}+\hat{S}_{2,x}+\hat{S}_{3,x})^2 + (\hat{S}_{1,y}+\hat{S}_{2,y}+\hat{S}_{3,y})^2 - \hat{S}_{1,x}^2 - \hat{S}_{1,y}^2 - \hat{S}_{2,x}^2 - \hat{S}_{2,y}^2 - \hat{S}_{3,x}^2 - \hat{S}_{3,y}^2\right]$
$= \frac{1}{2}\hat{\boldsymbol{S}}_{1+2+3}^2 - \frac{1}{2}\hat{S}_{1+2+3,z}^2 - \frac{3}{4}$.

Here $\hat{\boldsymbol{S}}_{1+2+3} = \hat{\boldsymbol{S}}_1 + \hat{\boldsymbol{S}}_2 + \hat{\boldsymbol{S}}_3$ is the total spin. And we have used the fact that $\hat{S}_{i,a}^2 = \frac{1}{4}$ for spin-1/2 moments. Therefore the eigenstates of total spin and total S_z, $|S_{1+2+3}, S_{1+2+3,z}\rangle$ are eigenstates of $\hat{H}$. These states have been built in Homework #5 Problem 4(b), and are also listed above in (a).

Eigenvalue= $\frac{1}{2}\cdot\frac{3}{2}(\frac{3}{2}+1) - \frac{1}{2}\cdot(\pm\frac{3}{2})^2 - \frac{3}{4} = 0$, for $|S_{1+2+3}=\frac{3}{2}, S_{1+2+3,z}=\pm\frac{3}{2}\rangle$ states.

Eigenvalue= $\frac{1}{2}\cdot\frac{3}{2}(\frac{3}{2}+1) - \frac{1}{2}\cdot(\pm\frac{1}{2})^2 - \frac{3}{4} = 1$, for $|S_{1+2+3}=\frac{3}{2}, S_{1+2+3,z}=\pm\frac{1}{2}\rangle$ states.

Eigenvalue= $\frac{1}{2}\cdot\frac{1}{2}(\frac{1}{2}+1) - \frac{1}{2}\cdot(\pm\frac{1}{2})^2 - \frac{3}{4} = -\frac{1}{2}$, for $|S_{1+2+3}=\frac{1}{2}, S_{1+2+3,z}=\pm\frac{1}{2}\rangle$ states.

Method #2:

$\hat{H} = \frac{1}{2}(\hat{S}_{1,+}\hat{S}_{2,-} + \hat{S}_{1,-}\hat{S}_{2,+}) + \frac{1}{2}(\hat{S}_{2,+}\hat{S}_{3,-} + \hat{S}_{2,-}\hat{S}_{3,+}) + \frac{1}{2}(\hat{S}_{3,+}\hat{S}_{1,-} + \hat{S}_{3,-}\hat{S}_{1,+})$. So it conserves total S_z. Divide the 8-dimensional Hilbert space into subspaces of fixed total S_z.

In the $\hat{S}_{1+2+3,z} = \frac{3}{2}$ space, with basis $|\uparrow\uparrow\uparrow\rangle$, $\hat{H}$ is (0).

In the $\hat{S}_{1+2+3,z} = -\frac{3}{2}$ space, with basis $|\downarrow\downarrow\downarrow\rangle$, $\hat{H}$ is (0).

In the $\hat{S}_{1+2+3,z} = \frac{1}{2}$ space, with basis $(|\downarrow\uparrow\uparrow\rangle, |\uparrow\downarrow\uparrow\rangle, |\uparrow\uparrow\downarrow\rangle)$, $\hat{H}$ is $\frac{1}{2}\begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix}$.

In the $\hat{S}_{1+2+3,z} = -\frac{1}{2}$ space, with basis $(|\uparrow\downarrow\downarrow\rangle, |\downarrow\uparrow\downarrow\rangle, |\downarrow\downarrow\uparrow\rangle)$, $\hat{H}$ is $\frac{1}{2}\begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix}$.

The 3×3 matrix above has eigenvalue 1 with eigenvector $\frac{1}{\sqrt{3}}\begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}$, and eigenvalue $-\frac{1}{2}$ with eigenvector $\frac{1}{\sqrt{3}}\begin{pmatrix} 1 \\ e^{2\pi \mathbb{i}/3} \\ e^{-2\pi \mathbb{i}/3} \end{pmatrix}$ and $\frac{1}{\sqrt{3}}\begin{pmatrix} 1 \\ e^{-2\pi \mathbb{i}/3} \\ e^{2\pi \mathbb{i}/3} \end{pmatrix}$.

(d) Answer #1: $\hat{H}$ has time-reversal symmetry (each term is a product of even-number of spin operators), and the system consists of odd-number of spin-1/2 (so $\hat{\mathcal{T}}^2 = -\mathbb{1}$), so there must be Kramers degeneracy, all energy levels are at least 2-fold degenerate.

Answer #2: consider $\hat{U} = \exp(-\mathbb{i}\pi \hat{S}_{1+2+3,y})$, then $\hat{U}\hat{S}_{i,z}\hat{U}^\dagger = -\hat{S}_{i,z}$, $\hat{U}\hat{S}_{i,x}\hat{U}^\dagger = -\hat{S}_{i,x}$, $\hat{U}\hat{S}_{i,y}\hat{U}^\dagger = +\hat{S}_{i,y}$. So $\hat{U}\hat{H}\hat{U}^\dagger = \hat{H}$, but $\hat{U}\hat{S}_z\hat{U}^\dagger = -\hat{S}_z$, namely $\hat{U}$ does not change $\hat{H}$ eigenvalue, but changes sign of $\hat{S}_z$ eigenvalue. $\hat{S}_z$ eigenvalues are nonzero, therefore $\hat{H}$ eigenvalue must be at least 2-fold degenerate.

Problem 3. (5 points) $\Gamma_{1,2,3,4}$ are 4×4 traceless hermitian matricies, $(\Gamma_i)^\dagger = \Gamma_i$, $\mathrm{Tr}(\Gamma_i) = 0$. And $(\Gamma_i)^2 = \mathbb{1}_{4\times 4}$ are identity matrix. And $[\Gamma_1, \Gamma_3] = [\Gamma_1, \Gamma_4] = [\Gamma_2, \Gamma_3]$ $= [\Gamma_2, \Gamma_4] = \{\Gamma_1, \Gamma_2\} = \{\Gamma_3, \Gamma_4\} = 0$. *Solve the eigenvalues of* $((a_1\Gamma_1 + a_2\Gamma_2) + (a_3\Gamma_3 + a_4\Gamma_4))$, *where* $a_{1,2,3,4}$ *are real numbers.* [Hint: you may define $\hat{S}_{1,z} = \frac{\Gamma_1}{2}$, $\hat{S}_{1,x} = \frac{\Gamma_2}{2}$, $\hat{S}_{2,z} = \frac{\Gamma_3}{2}$, $\hat{S}_{2,x} = \frac{\Gamma_4}{2}$, and make analogy to a problem with two spin-1/2]

Solution

$(a_1\Gamma_1 + a_2\Gamma_2)^2 = (a_1^2 + a_2^2)\mathbb{1}_{4\times 4}$, $(a_3\Gamma_3 + a_4\Gamma_4)^2 = (a_3^2 + a_4^2)\mathbb{1}_{4\times 4}$.

Therefore the 4×4 traceless hermitian matrix $a_1\Gamma_1 + a_2\Gamma_2$ has eigenvalues $\pm\sqrt{a_1^2 + a_2^2}$ (each is 2-fold degenerate), and $a_3\Gamma_3 + a_4\Gamma_4$ has eigenvalues $\pm\sqrt{a_3^2 + a_4^2}$ (each is 2-fold degenerate).

The eigenvalues of $(a_1\Gamma_1 + a_2\Gamma_2) + (a_3\Gamma_3 + a_4\Gamma_4)$ are $+\sqrt{a_1^2 + a_2^2} + \sqrt{a_3^2 + a_4^2}$, $+\sqrt{a_1^2 + a_2^2} - \sqrt{a_3^2 + a_4^2}$, $-\sqrt{a_1^2 + a_2^2} + \sqrt{a_3^2 + a_4^2}$, $-\sqrt{a_1^2 + a_2^2} - \sqrt{a_3^2 + a_4^2}$.

(Not required) To be rigorous, we need to prove all the above four combinations appear. Define $U_1 = \mathbb{i}\Gamma_1\Gamma_2$, $U_2 = \mathbb{i}\Gamma_3\Gamma_4$. It is easy to check that $(U_1)^\dagger = U_1$, $(U_2)^\dagger = U_2$, and $U_1^2 = U_2^2 = \mathbb{1}_{4\times 4}$, and $U_1U_2 = U_2U_1$. So $U_{1,2}$ are both unitary matrices, and commute.

$U_1\Gamma_1U_1^\dagger = -\Gamma_1$, $U_1\Gamma_2U_1^\dagger = -\Gamma_2$, $U_1\Gamma_3U_1^\dagger = \Gamma_3$, $U_1\Gamma_4U_1^\dagger = \Gamma_4$.

$U_2\Gamma_1U_2^\dagger = \Gamma_1$, $U_2\Gamma_2U_2^\dagger = \Gamma_2$, $U_2\Gamma_3U_2^\dagger = -\Gamma_3$, $U_2\Gamma_4U_2^\dagger = -\Gamma_4$.

Since $[a_1\Gamma_1 + a_2\Gamma_2, a_3\Gamma_3 + a_4\Gamma_4] = 0$, we can find their simultaneous eigenvector $\vec{v}$, with

$(a_1\Gamma_1 + a_2\Gamma_2)\cdot\vec{v} = \lambda_1\vec{v}$, $(a_3\Gamma_3 + a_4\Gamma_4)\cdot\vec{v} = \lambda_2\vec{v}$. Then

$U_1\vec{v}$ has eigenvalue $-\lambda_1$ for $a_1\Gamma_1 + a_2\Gamma_2$, eigenvalue λ_2 for $a_3\Gamma_3 + a_4\Gamma_4$;

$U_2\vec{v}$ has eigenvalue λ_1 for $a_1\Gamma_1 + a_2\Gamma_2$, eigenvalue $-\lambda_2$ for $a_3\Gamma_3 + a_4\Gamma_4$;

$U_1U_2\vec{v}$ has eigenvalue $-\lambda_1$ for $a_1\Gamma_1 + a_2\Gamma_2$, eigenvalue $-\lambda_2$ for $a_3\Gamma_3 + a_4\Gamma_4$.

The following analogy to spin-1/2 is not really necessary. Define $\hat{S}_{1,z} = \frac{\Gamma_1}{2}$, $\hat{S}_{1,x} = \frac{\Gamma_2}{2}$, $\hat{S}_{2,z} = \frac{\Gamma_3}{2}$, $\hat{S}_{2,x} = \frac{\Gamma_4}{2}$, and $\hat{S}_{1,y} = \mathbb{i}[\hat{S}_{1,x}, \hat{S}_{1,z}] = \frac{\mathbb{i}}{2}\Gamma_2\Gamma_1$, $\hat{S}_{2,y} = \mathbb{i}[\hat{S}_{2,x}, \hat{S}_{2,z}] = \frac{\mathbb{i}}{2}\Gamma_4\Gamma_3$. It is easy to check that they satisfy the commutation relations of two spins, $[\hat{S}_{i,a}, \hat{S}_{j,b}] = \delta_{i,j}\sum_c \epsilon_{abc}\hat{S}_{i,c}$. And because $\hat{S}_{i,z}$ can only have eigenvalues $\pm\frac{1}{2}$, they are two spin-1/2 moments. Then $a_1\Gamma_1 + a_2\Gamma_2 + a_3\Gamma_3 + a_4\Gamma_4$ is $(2a_2, 0, 2a_1)\cdot\hat{\boldsymbol{S}}_1 + (2a_4, 0, 2a_3)\cdot\hat{\boldsymbol{S}}_2$, which looks like two decoupled spin-1/2 under different Zeeman field.

Problem 4. (30 points) Consider three fermion modes $\hat{f}_{1,2,3}$. They satisfy $\{\hat{f}_i, \hat{f}_j^\dagger\} = \delta_{ij}$. Let $\hat{H}_0 = E_0\cdot(\hat{n}_1 - \hat{n}_3)$. Here $\hat{n}_i = \hat{f}_i^\dagger\hat{f}_i$, $E_0 > 0$ is a real number. The occupation basis $|n_1, n_2, n_3\rangle = (\hat{f}_1^\dagger)^{n_1}(\hat{f}_2^\dagger)^{n_2}(\hat{f}_3^\dagger)^{n_3}|\text{vac}\rangle$ are orthonormal eigenstates of $\hat{H}_0$ with eigenvalue $E_0\cdot(n_1 - n_3)$, where $n_{1,2,3} = 0$ or 1 are eigenvalues of $\hat{n}_{1,2,3}$, $|\text{vac}\rangle$ is the normalized "vacuum".

(a) (8pts) Add a time-independent perturbation, $\hat{V} = -t\cdot((\hat{f}_1^\dagger\hat{f}_2 + \hat{f}_2^\dagger\hat{f}_3) + (\hat{f}_2^\dagger\hat{f}_1 + \hat{f}_3^\dagger\hat{f}_2))$. Here t is a real "small parameter". *Solve the approximate eigenvalues of $\hat{H} = \hat{H}_0 + \hat{V}$ up to 2nd order of t in the entire Fock space.* [Hint: use perturbation theory, or solve exact eigenvalues of $\hat{H}$ and expand them to 3rd order of t, note $\hat{H}$ preserves total particle number, some facts about angular momentum might help]

(b) (8pts) Consider perturbation $\hat{V}' = -t\cdot((\hat{f}_1^\dagger\hat{f}_2 + \hat{f}_2^\dagger\hat{f}_3) + (\hat{f}_2^\dagger\hat{f}_1 + \hat{f}_3^\dagger\hat{f}_2) + (\hat{f}_1\hat{f}_3 + \hat{f}_3^\dagger\hat{f}_1^\dagger))$. *Solve the approximate eigenvalues of $\hat{H}' = \hat{H}_0 + \hat{V}'$ up to 2nd order of t in the entire Fock space.* [Hint: $\hat{H}'$ does NOT preserve total particle number, but preserves particle number parity; high-order degenerate perturbation theory may be avoided by changing to the eigenbasis of 1st order secular equation]

(c) (8pts*) *Solve the approximate eigenvalues of $\hat{H}' = \hat{H}_0 + \hat{V}'$ in (b) up to 3rd order of t in the entire Fock space.* [Hint: you can get these directly if (b) is done carefully]

(d) (4pts**) *Solve the eigenvalues of $\hat{H}'$ in (c) exactly.* [Hint: some previous results may be useful]

(e) (2pts***) You may have noticed that the (approximate) eigenvalues in (b)(c)(d) are 2-fold degenerate. *Prove this by first proving the following statement in [...], and then find the unitary $\hat{U}$ and hermitian $\hat{P}$.* [If operators $\hat{H}'$ and $\hat{P}$ are both hermitian, $\hat{P}^2 = \mathbb{1}$, and there is a unitary operator $\hat{U}$ so that $\hat{U}\hat{H}'\hat{U}^\dagger = \hat{H}'$ and $\hat{U}\hat{P}\hat{U}^\dagger = -\hat{P}$. Then the eigenvalues of $\hat{H}'$ must be at least 2-fold degenerate.]

Solution

For reasons to be explained later, choose the basis $|\psi_i\rangle$ $(i = 1, \ldots, 8)$ for the Fock space as $(|\text{vac}\rangle,\ \hat{f}_1^\dagger\hat{f}_3^\dagger|\text{vac}\rangle = -\hat{f}_2\hat{f}_1^\dagger\hat{f}_2^\dagger\hat{f}_3^\dagger|\text{vac}\rangle,\ \hat{f}_1^\dagger\hat{f}_2^\dagger|\text{vac}\rangle = \hat{f}_3\hat{f}_1^\dagger\hat{f}_2^\dagger\hat{f}_3^\dagger|\text{vac}\rangle,\ \hat{f}_2^\dagger\hat{f}_3^\dagger|\text{vac}\rangle = \hat{f}_1\hat{f}_1^\dagger\hat{f}_2^\dagger\hat{f}_3^\dagger|\text{vac}\rangle,$ $-\hat{f}_1^\dagger\hat{f}_2^\dagger\hat{f}_3^\dagger|\text{vac}\rangle,\ \hat{f}_2^\dagger|\text{vac}\rangle,\ \hat{f}_1^\dagger|\text{vac}\rangle,\ \hat{f}_3^\dagger|\text{vac}\rangle)$.

(a) Method #1: directly use series expansion result,

$\hat{H}$ under the above basis is block-diagonal within subspaces of fixed particle number,

$$\hat{H} = \begin{pmatrix} 0 &&&&&&& \\ & 0 &&&&&& \\ && E_0 &&&&& \\ &&& -E_0 &&&& \\ &&&& 0 &&& \\ &&&&& 0 && \\ &&&&&& E_0 & \\ &&&&&&& -E_0 \end{pmatrix} + \begin{pmatrix} 0 &&&&&&& \\ & 0 & -t & -t &&&& \\ & -t & 0 & 0 &&&& \\ & -t & 0 & 0 &&&& \\ &&&& 0 &&& \\ &&&&& 0 & -t & -t \\ &&&&& -t & 0 & 0 \\ &&&&& -t & 0 & 0 \end{pmatrix}.$$

Note that the top-left 4×4 diagonal block is the same as the bottom-right 4×4 diagonal block. So every eigenvalue is 2-fold degenerate. Directly use the non-degenerate second order perturbation result, $E_{1,5} = 0$ (exact);

$E_{2,6} \approx 0 + \frac{t^2}{0-E_0} + \frac{t^2}{0-(-E_0)} = 0$ (this is actually exact);

$E_{3,7} \approx E_0 + \frac{t^2}{E_0-0} = E_0 + \frac{t^2}{E_0}$;

$E_{4,8} \approx -E_0 + \frac{t^2}{-E_0-0} = -E_0 - \frac{t^2}{E_0}$.

Method #2: diagonalize this "bilinear operator" exactly,

$$\hat{H} = (\hat{f}_1^\dagger, \hat{f}_2^\dagger, \hat{f}_3^\dagger) \cdot \left[E_0 \cdot \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix} + (-t) \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \right] \cdot \begin{pmatrix} \hat{f}_1 \\ \hat{f}_2 \\ \hat{f}_3 \end{pmatrix}.$$

The 3×3 matrix is the spin-1 operator, $E_0\hat{S}_z + (-\sqrt{2}t)\hat{S}_x$, under S_z basis. Similar to Homework #2 Problem 4(d) and Midterm Problem 3(e), we can use a unitary transformation to "rotate" this bilinear operator's coefficient matrix into $\sqrt{E_0^2+(-\sqrt{2}t)^2}\hat{S}_z$.

So $\hat{H}$ is related to $\sqrt{E_0^2+2t^2}(\hat{n}_1-\hat{n}_3)$ by a unitary transformation. The exact eigenvalues are 0 (4-fold), $\sqrt{E_0^2+2t^2}\approx E_0+\frac{t^2}{E_0}$ (2-fold), $-\sqrt{E_0^2+2t^2}\approx -E_0-\frac{t^2}{E_0}$ (2-fold).

Method #3: use unitary transformations,

Define $\hat{V}_{+1}\equiv -t\cdot(\hat{f}_1^\dagger\hat{f}_2+\hat{f}_2^\dagger\hat{f}_3)$, $\hat{V}_{-1}\equiv -t\cdot(\hat{f}_2^\dagger\hat{f}_1+\hat{f}_3^\dagger\hat{f}_2)$. Then $\hat{V}=\hat{V}_{+1}+\hat{V}_{-1}$, $(\hat{V}_{\pm1})^\dagger=\hat{V}_{\mp1}$, $[\hat{H}_0,\hat{V}_{\pm1}]=\pm E_0\cdot\hat{V}_{\pm1}$. The perturbation contains only "off-diagonal" terms.

Define unitary operator $e^{\mathbb{i}\hat{S}}$ with $\mathbb{i}\hat{S}=\frac{\hat{V}_{+1}-\hat{V}_{-1}}{E_0}$. Then $[\mathbb{i}\hat{S},\hat{H}_0]=-\hat{V}$. This unitary transformation, $e^{\mathbb{i}\hat{S}}(\hat{H}_0+\hat{V})e^{-\mathbb{i}\hat{S}}$, will produce accurate "diagonal terms" up to $O(t^3)$.

For later problem (c), keep up to $O(t^3)$ terms,

$e^{\mathbb{i}\hat{S}}(\hat{H}_0+\hat{V})e^{-\mathbb{i}\hat{S}}=\hat{H}_0+(1-\frac{1}{2})[\mathbb{i}\hat{S},\hat{V}]+(\frac{1}{2}-\frac{1}{6})[\mathbb{i}\hat{S},[\mathbb{i}\hat{S},\hat{V}]+O(t^4)$.

Use $[\hat{f}_i^\dagger\hat{f}_j,\hat{f}_k^\dagger]=\delta_{jk}\hat{f}_i^\dagger$, and $[\hat{f}_i^\dagger\hat{f}_j,\hat{f}_k]=-\delta_{ik}\hat{f}_j^\dagger$.

$[\mathbb{i}\hat{S},\hat{V}]=\frac{2}{E_0}[\hat{V}_{+1},\hat{V}_{-1}]=\frac{2t^2}{E_0}(\hat{f}_1^\dagger\hat{f}_1-\hat{f}_2^\dagger\hat{f}_2+\hat{f}_2^\dagger\hat{f}_2-\hat{f}_3^\dagger\hat{f}_3)=\frac{2t^2}{E_0}(\hat{n}_1-\hat{n}_3)=\frac{2t^2}{E_0^2}\hat{H}_0$.

Then $[\mathbb{i}\hat{S},[\mathbb{i}\hat{S},\hat{V}]]=[\mathbb{i}\hat{S},\frac{2t^2}{E_0^2}\hat{H}_0]=-\frac{2t^2}{E_0^2}\hat{V}$.

The "diagonal terms" up to $O(t^3)$ is $\hat{H}_0+(1-\frac{1}{2})\frac{2t^2}{E_0^2}\hat{H}_0=(E_0+\frac{t^2}{E_0})(\hat{n}_1-\hat{n}_3)$.

So transformed occupation basis, $e^{\mathbb{i}\hat{S}}|n_1,n_2,n_3\rangle$, are approximate eigenstates with eigenvalues $(E_0+\frac{t^2}{E_0})(n_1-n_3)$, $n_{1,2,3}=0$ or 1.

(b)(c) Method #1: use series expansion method,

Under the above Fock space basis,

$$\hat{H}'=\begin{pmatrix}0&&&&&&&\\&0&&&&&&\\&&E_0&&&&&\\&&&-E_0&&&&\\&&&&0&&&\\&&&&&0&&\\&&&&&&E_0&\\&&&&&&&-E_0\end{pmatrix}+\begin{pmatrix}0&t&&&&&&\\t&0&-t&-t&&&&\\&-t&0&0&&&&\\&-t&0&0&&&&\\&&&&0&t&&\\&&&&t&0&-t&-t\\&&&&&-t&0&0\\&&&&&-t&0&0\end{pmatrix}.$$

It is still block-diagonal, because $\hat{H}'$ preserves particle number parity, and the first four basis have even-number of particles, last four basis have odd-number of particles.

The two identical 4×4 diagonal blocks, $\begin{pmatrix}0&&&\\&0&&\\&&E_0&\\&&0&-E_0\end{pmatrix}+\begin{pmatrix}0&t&0&0\\t&0&-t&-t\\0&-t&0&0\\0&-t&0&0\end{pmatrix}$, are solved as follows.

Method #1.1: directly use degenerate perturbation theory,

For the first two degenerate levels of $\hat{H}_0$, define $\hat{P} = \begin{pmatrix} 1 & & & \\ & 1 & & \\ & & 0 & \\ & & & 0 \end{pmatrix}$, $\hat{Q} = \mathbb{1}_{4\times 4} - \hat{P}$, $\hat{G} = \begin{pmatrix} 0 & & & \\ & 0 & & \\ & & \frac{1}{E-E_0} & \\ & & & \frac{1}{E+E_0} \end{pmatrix}$, the secular equation up to 3rd order is $\hat{P}\hat{V}\hat{P}+\hat{P}\hat{V}\hat{G}\hat{V}\hat{P}+\hat{P}\hat{V}\hat{G}\hat{V}\hat{G}\hat{V}\hat{P}$ $= \begin{pmatrix} 0, & t \\ t, & \frac{t^2}{E-E_0} + \frac{t^2}{E+E_0} \end{pmatrix} = \begin{pmatrix} 0, & t \\ t, & \frac{2Et^2}{E^2-E_0^2} \end{pmatrix}$. This is $\frac{Et^2}{E^2-E_0^2}\sigma_0 - \frac{Et^2}{E^2-E_0^2}\sigma_3 + t\sigma_1$.
The eigenvalues of secular equation are $\frac{Et^2}{E^2-E_0^2} \pm \sqrt{t^2 + (\frac{Et^2}{E^2-E_0^2})^2}$.

Choose "+" sign, the first order approximation is then $E \approx t$, plug this back into the formula and expand to t^3 order, $E_{1,5} \approx t - \frac{t^3}{E_0^2}$.

Choose "−" sign, the first order approximation is then $E \approx -t$, plug this back into the formula and expand to t^3 order, $E_{2,6} \approx -t + \frac{t^3}{E_0^2}$.

The steps for the 3rd order perturbation results for non-degenerate levels are omitted here, they are still $E_{3,7} \approx E_0 + \frac{t^2}{E_0}$; $E_{4,8} \approx -E_0 - \frac{t^2}{E_0}$.

Method #1.2: first change to eigenbasis of 1st order secular equation,

the 1st order secular equation is $\begin{pmatrix} 0 & t & & \\ t & 0 & & \\ & & & \\ & & & \end{pmatrix}$. Define new basis $|\tilde{\psi}_1\rangle = \frac{1}{\sqrt{2}}(|\psi_1\rangle + |\psi_2\rangle)$, $|\tilde{\psi}_2\rangle = \frac{1}{\sqrt{2}}(|\psi_1\rangle - |\psi_2\rangle)$, then $\hat{H}_0$ does not change, but $\hat{V}'$ becomes $\begin{pmatrix} t & 0 & -\frac{t}{\sqrt{2}} & -\frac{t}{\sqrt{2}} \\ 0 & -t & \frac{t}{\sqrt{2}} & \frac{t}{\sqrt{2}} \\ -\frac{t}{\sqrt{2}} & \frac{t}{\sqrt{2}} & 0 & 0 \\ -\frac{t}{\sqrt{2}} & \frac{t}{\sqrt{2}} & 0 & 0 \end{pmatrix}$.

Redefine $\hat{\hat{H}}_0 = \begin{pmatrix} t & & & \\ & -t & & \\ & & E_0 & \\ & & & -E_0 \end{pmatrix}$, and $\hat{\hat{V}}' = \begin{pmatrix} 0 & 0 & -\frac{t}{\sqrt{2}} & -\frac{t}{\sqrt{2}} \\ 0 & 0 & \frac{t}{\sqrt{2}} & \frac{t}{\sqrt{2}} \\ -\frac{t}{\sqrt{2}} & \frac{t}{\sqrt{2}} & 0 & 0 \\ -\frac{t}{\sqrt{2}} & \frac{t}{\sqrt{2}} & 0 & 0 \end{pmatrix}$. $\hat{H}' = \hat{\hat{H}}_0 + \hat{\hat{V}}'$. We can now use non-degenerate perturbation theory. Because sign of $\hat{\hat{V}}'$ can be changed by unitary operator $\begin{pmatrix} 1 & & & \\ & 1 & & \\ & & -1 & \\ & & & -1 \end{pmatrix}$, while maintaining $\hat{\hat{H}}_0$, so $\hat{\hat{V}}'$ will only generate even-order perturbations. Up to 3rd order the approximate eigenvalues are

$E_{1,5} \approx t + \frac{t^2/2}{t-E_0} + \frac{t^2/2}{t-(-E_0)} = t + \frac{2t\cdot t^2/2}{t^2-E_0^2} \approx t - \frac{t^3}{E_0^2}$,
$E_{2,6} \approx -t + \frac{t^2/2}{-t-E_0} + \frac{t^2/2}{-t-(-E_0)} = -t + \frac{-2t\cdot t^2/2}{t^2-E_0^2} \approx -t + \frac{t^3}{E_0^2}$,
$E_{3,7} \approx E_0 + \frac{t^2/2}{E_0-t} + \frac{t^2/2}{E_0-(-t)} = E_0 + \frac{2E_0\cdot t^2/2}{E_0^2-t^2} \approx E_0 + \frac{t^2}{E_0}$,
$E_{4,8} \approx -E_0 + \frac{t^2/2}{-E_0-t} + \frac{t^2/2}{-E_0-(-t)} = -E_0 + \frac{-2E_0\cdot t^2/2}{E_0^2-t^2} \approx -E_0 - \frac{t^2}{E_0}$.

Method #2: use unitary transformations,

Define $\hat{V}_0 = -t\cdot(\hat{f}_1\hat{f}_3 + \hat{f}_3^\dagger\hat{f}_1^\dagger)$, then $\hat{V}' = \hat{V} + \hat{V}_0 = \hat{V}_{+1} + \hat{V}_{-1} + \hat{V}_0$, $[\hat{H}_0, \hat{V}_0] = 0$.

The unitary operator for removing "off-diagonal terms" is the same as that in (a), $e^{\mathbb{i}\hat{S}}$ with $\mathbb{i}\hat{S} = \frac{\hat{V}_{+1}-\hat{V}_{-1}}{E_0}$, $[\mathbb{i}\hat{S}, \hat{H}_0] = -\hat{V}_{+1} - \hat{V}_{-1}$.

$e^{\mathbb{i}\hat{S}}(\hat{H}_0 + \hat{V}')e^{-\mathbb{i}\hat{S}} = e^{\mathbb{i}\hat{S}}(\hat{H}_0 + \hat{V})e^{-\mathbb{i}\hat{S}} + e^{\mathbb{i}\hat{S}}\hat{V}_0 e^{-\mathbb{i}\hat{S}}$, the first term has been computed in (a) up to $O(t^3)$, $e^{\mathbb{i}\hat{S}}(\hat{H}_0 + \hat{V})e^{-\mathbb{i}\hat{S}} = (E_0 + \frac{t^2}{E_0})(\hat{n}_1 - \hat{n}_3) + O(t^4)$.

$e^{\mathbb{i}\hat{S}}\hat{V}_0 e^{-\mathbb{i}\hat{S}}$ up to $O(t^3)$ is $\hat{V}_0 + [\mathbb{i}\hat{S}, \hat{V}_0] + \frac{1}{2}[\mathbb{i}\hat{S}, [\mathbb{i}\hat{S}, \hat{V}_0]] + O(t^4)$.

$[\mathbb{i}\hat{S}, \hat{V}_0] = \frac{t^2}{E_0}[(\hat{f}_1^\dagger\hat{f}_2 + \hat{f}_2^\dagger\hat{f}_3) - (\hat{f}_2^\dagger\hat{f}_1 + \hat{f}_3^\dagger\hat{f}_2), (\hat{f}_1\hat{f}_3 + \hat{f}_3^\dagger\hat{f}_1^\dagger)] = \frac{t^2}{E_0}(-\hat{f}_2\hat{f}_3 + \hat{f}_2^\dagger\hat{f}_1^\dagger - \hat{f}_3^\dagger\hat{f}_2^\dagger + \hat{f}_1\hat{f}_2)$.

$[\mathbb{i}\hat{S}, [\mathbb{i}\hat{S}, \hat{V}_0]] = -\frac{t^3}{E_0^2}(-\hat{f}_3^\dagger\hat{f}_1^\dagger - \hat{f}_1\hat{f}_3 - \hat{f}_1\hat{f}_3 - \hat{f}_3^\dagger\hat{f}_1^\dagger)$.

So "diagonal terms" (commutes with $\hat{H}_0$) up to $O(t^3)$ is $(E_0 + \frac{t^2}{E_0})(\hat{n}_1 - \hat{n}_3) - (t - \frac{t^3}{E_0^2})(\hat{f}_1\hat{f}_3 + \hat{f}_3^\dagger\hat{f}_1^\dagger)$.

In the first four basis, this is $\begin{pmatrix} 0 & (t-\frac{t^3}{E_0^3}) & & \\ (t-\frac{t^3}{E_0^3}) & 0 & & \\ & & E_0 + \frac{t^2}{E_0} & \\ & & & -E_0 - \frac{t^2}{E_0} \end{pmatrix}$. Further diagonalize the top-left 2×2 block (secular equation), we get the approximate eigenvalues, $E_{1,5} \approx t - \frac{t^3}{E_0^2}$, $E_{2,6} \approx -t + \frac{t^3}{E_0^2}$, $E_{3,7} \approx E_0 + \frac{t^2}{E_0}$, $E_{4,8} \approx -E_0 - \frac{t^2}{E_0}$.

(d) Consider the 4×4 matrix in Method #1.2 of (b)(c). It is $\frac{E_0+t}{2}\sigma_0\otimes\sigma_3 + \frac{t}{\sqrt{2}}\sigma_2\otimes\sigma_2 + \frac{t-E_0}{2}\sigma_3\otimes\sigma_3 - \frac{t}{\sqrt{2}}\sigma_1\otimes\sigma_3$.

These four 4×4 matrices satisfy the conditions in Problem 3.

So the exact eigenvalues are $+\lambda_1 + \lambda_2$, $+\lambda_1 - \lambda_2$, $-\lambda_1 + \lambda_2$, $-\lambda_1 - \lambda_2$, with
$\lambda_1 = \sqrt{(\frac{E_0+t}{2})^2 + (\frac{t}{\sqrt{2}})^2} = \frac{E_0}{2}\sqrt{1 + \frac{2t}{E_0} + \frac{3t^2}{E_0^2}} \approx \frac{E_0}{2}(1 + \frac{t}{E_0} + \frac{t^2}{E_0^2} - \frac{t^3}{E_0^3}) + O(t^4)$,
$\lambda_2 = \sqrt{(\frac{t-E_0}{2})^2 + (-\frac{t}{\sqrt{2}})^2} = \frac{E_0}{2}\sqrt{1 - \frac{2t}{E_0} + \frac{3t^2}{E_0^2}} \approx \frac{E_0}{2}(1 - \frac{t}{E_0} + \frac{t^2}{E_0^2} + \frac{t^3}{E_0^3}) + O(t^4)$.

(e)

Under the condition that $[\hat{H}', \hat{P}] = 0$ (forgot to state in the problem).

Consider an eigenstate $|\hat{H}'=E,\hat{P}=\lambda\rangle$ of both $\hat{H}'$ and $\hat{P}$. Because $\hat{P}^2=\mathbb{1}$, $\lambda=\pm 1\neq 0$. Then $\hat{H}'\hat{U}|\hat{H}'=E,\hat{P}=\lambda\rangle=\hat{U}\hat{H}'\hat{U}^\dagger\hat{U}|\hat{H}'=E,\hat{P}=\lambda\rangle=\hat{U}\hat{H}'|\hat{H}'=E,\hat{P}=\lambda\rangle$ $=E\cdot\hat{U}|\hat{H}'=E,\hat{P}=\lambda\rangle$, and $\hat{P}\hat{U}|\hat{H}'=E,\hat{P}=\lambda\rangle=-\hat{U}\hat{P}\hat{U}^\dagger\hat{U}|\hat{H}'=E,\hat{P}=\lambda\rangle$ $=-\hat{U}\hat{P}|\hat{H}'=E,\hat{P}=\lambda\rangle=-\lambda\cdot\hat{U}|\hat{H}'=E,\hat{P}=\lambda\rangle$.

Therefore $\hat{U}|\hat{H}'=E,\hat{P}=\lambda\rangle=|\hat{H}'=E,\hat{P}=-\lambda\rangle$ and is different from $|\hat{H}'=E,\hat{P}=\lambda\rangle$, because $\lambda\neq 0$. So the eigenvalue E eigenstate of $\hat{H}'$ must be at least 2-fold degenerate.

Under the above basis for Fock space, we can choose

$$\hat{U}=\begin{pmatrix} & & & & 1 & & & \\ & & & & & 1 & & \\ & & & & & & 1 & \\ & & & & & & & 1 \\ 1 & & & & & & & \\ & 1 & & & & & & \\ & & 1 & & & & & \\ & & & 1 & & & & \end{pmatrix},\ \hat{P}=\begin{pmatrix} 1 & & & & & & & \\ & 1 & & & & & & \\ & & 1 & & & & & \\ & & & 1 & & & & \\ & & & & -1 & & & \\ & & & & & -1 & & \\ & & & & & & -1 & \\ & & & & & & & -1 \end{pmatrix}.$$

$\hat{P}$ is the fermion number parity operator,

$$\hat{P}=(-1)^{\sum_i \hat{n}_i}=\begin{cases} +1, & \text{even particle number states;} \\ -1, & \text{odd particle number states.} \end{cases}$$

$\hat{U}$ corresponds to the following (particle-hole transformation)$\times$(a unitary transform of creation/annihilation operator basis), $\hat{U}\hat{f}_1^\dagger\hat{U}^\dagger=\hat{f}_3$, $\hat{U}\hat{f}_2^\dagger\hat{U}^\dagger=-\hat{f}_2$, $\hat{U}\hat{f}_3^\dagger\hat{U}^\dagger=\hat{f}_1$. It should be easy to see that $\hat{U}\hat{H}'\hat{U}^\dagger=\hat{H}'$, and $\hat{U}\hat{P}\hat{U}^\dagger=-\hat{P}$.

The last four basis of Fock space are related to the first four basis by this unitary transform, $|\psi_{i+4}\rangle=\hat{U}|\psi_i\rangle$ for $i=1,2,3,4$, if we define $\hat{U}|\text{vac}\rangle=-\hat{f}_1^\dagger\hat{f}_2^\dagger\hat{f}_3^\dagger|\text{vac}\rangle$.

The explicit form of $\hat{U}$ in terms of creation/annihilation operators is (not required),

$$\hat{U}=(-1)^{\hat{n}_3}\exp\left[-\mathbb{i}\tfrac{\pi}{2}(\hat{f}_1^\dagger,\hat{f}_3^\dagger)\cdot\tfrac{\sigma_2}{2}\cdot\begin{pmatrix}\hat{f}_1\\ \hat{f}_3\end{pmatrix}\right]\cdot(-1)^{\hat{n}_2}\cdot(\hat{f}_3+\hat{f}_3^\dagger)(\hat{f}_2+\hat{f}_2^\dagger)(\hat{f}_1+\hat{f}_1^\dagger).$$