

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: $\exp(\hat{A}) \cdot \hat{B} \cdot \exp(-\hat{A}) = \hat{B} + \sum_{n=1}^{+\infty} \frac{1}{n!} \underbrace{[\hat{A}, [\hat{A}, \dots [\hat{A}, \hat{B}] \dots]]}_{n\text{-fold commutator}}]$.
- Spin (angular momentum) operators satisfy $[\hat{S}_a, \hat{S}_b] = i \sum_c \epsilon_{abc} \hat{S}_c$. ($a, b, c = x, y, z$)
 - $\hat{S}^2 \equiv \sum_a \hat{S}_a^2$ commutes with $\hat{S}_{x,y,z}$. Basis $|S, m\rangle$ satisfy, $\hat{S}_z|S, m\rangle = m|S, m\rangle$,
 $\hat{S}^2|S, m\rangle = S(S+1)|S, m\rangle$. $2S$ is non-negative integer, $m = -S, -S+1, \dots, S$.
 - Ladder operators $\hat{S}_{\pm} \equiv \hat{S}_x \pm i\hat{S}_y$, and $[\hat{S}_z, \hat{S}_{\pm}] = \pm\hat{S}_{\pm}$, and
 $\hat{S}_{\pm}|S, S_z = m\rangle = \sqrt{(S \mp m)(S \pm m + 1)}|S, S_z = m \pm 1\rangle$.
 - $e^{-i\theta \mathbf{n} \cdot \hat{\mathbf{S}}} \cdot \hat{S}_a \cdot e^{i\theta \mathbf{n} \cdot \hat{\mathbf{S}}} = \sum_b \hat{S}_b \cdot [R_{\mathbf{n}}(\theta)]_{ba}$. $SO(3)$ matrix for rotation around axis \mathbf{n}
by angle θ is $[R_{\mathbf{n}}(\theta)]_{ab} = n_a n_b + \cos \theta (\delta_{ab} - n_a n_b) - \sin \theta \sum_c \epsilon_{abc} n_c$, here \mathbf{n} is 3D
unit-length real vector, $\mathbf{n} \cdot \hat{\mathbf{S}} \equiv n_x \hat{S}_x + n_y \hat{S}_y + n_z \hat{S}_z$.
 - $\hat{S}_i \cdot \hat{S}_j \equiv \hat{S}_{iz} \hat{S}_{jz} + \hat{S}_{ix} \hat{S}_{jx} + \hat{S}_{iy} \hat{S}_{jy} = \hat{S}_{iz} \hat{S}_{jz} + \frac{1}{2}(\hat{S}_{i+} \hat{S}_{j-} + \hat{S}_{i-} \hat{S}_{j+})$.
- Spin-1/2: $\hat{S}_a = \sigma_a/2$ under the \hat{S}_z eigenbasis ($a = x, y, z$).
 Pauli matrices σ_a are $\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$, $\sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$, $\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$. $\{\sigma_a, \sigma_b\} = 2\delta_{ab}\mathbb{1}$.
 $\exp(-i\theta \mathbf{n} \cdot \boldsymbol{\sigma}) = \cos(\theta)\mathbb{1} - i \sin(\theta)(\mathbf{n} \cdot \boldsymbol{\sigma})$. $|\hat{S}_z = \pm \frac{1}{2}\rangle$ are denoted by $|\uparrow\rangle$ and $|\downarrow\rangle$.
- Spin-1: $\hat{S}_x = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}$, $\hat{S}_y = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix}$, $\hat{S}_z = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}$, under the \hat{S}_z eigenbasis.
- The D_3 group: $\{(C_3)^{(n \bmod 3)}(\sigma)^{(m \bmod 2)} | C_3^3 = \sigma^2 = C_3 \sigma C_3 \sigma = \mathbb{1}\}$.
 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, $\hat{\mathbf{S}}_1$ and $\hat{\mathbf{S}}_2$. They satisfy $[\hat{S}_{i,a}, \hat{S}_{j,b}] = \delta_{i,j} \sum_c i\epsilon_{abc} \hat{S}_{i,c}$ (here a, b, c label x, y, z components), $\hat{\mathbf{S}}_1^2 = \hat{\mathbf{S}}_2^2 = 1 \cdot (1 + 1) = 2$. 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 $\hat{H}_0 = -J \cdot \hat{\mathbf{S}}_1 \cdot \hat{\mathbf{S}}_2$. Here $J > 0$. [Hint: \hat{H}_0 is related to $(\hat{\mathbf{S}}_1 + \hat{\mathbf{S}}_2)^2$]

(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 $\exp[-i\theta \cdot (\hat{S}_{1,z} - \hat{S}_{2,z})] \cdot \hat{\chi}_z \cdot \exp[i\theta \cdot (\hat{S}_{1,z} - \hat{S}_{2,z})]$. θ 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 $|\psi(t)\rangle = e^{-i\hat{H}t/\hbar}|\psi(t=0)\rangle$. 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 $\hat{U}_I(t) = e^{i\hat{H}_0 t/\hbar}e^{-i\hat{H}t/\hbar}$; 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).

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

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).

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

This can also be proved by $\hat{\chi}_z = \frac{1}{2}(i\hat{S}_{1,+}\hat{S}_{2,-} - i\hat{S}_{1,-}\hat{S}_{2,+})$, 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,

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

$$\begin{aligned} & \text{Then } \exp[-i\theta \cdot (\hat{S}_{1,z} - \hat{S}_{2,z})] \cdot \hat{\chi}_z \cdot \exp[i\theta \cdot (\hat{S}_{1,z} - \hat{S}_{2,z})] \\ &= (\hat{S}_{1,x}\cos\theta + \hat{S}_{1,y}\sin\theta)(\hat{S}_{2,y}\cos\theta + \hat{S}_{2,x}\sin\theta) - (\hat{S}_{1,y}\cos\theta - \hat{S}_{1,x}\sin\theta)(\hat{S}_{2,x}\cos\theta - \hat{S}_{2,y}\sin\theta) \\ &= \cos(2\theta)\hat{\chi}_z + \sin(2\theta)(\hat{S}_{1,x}\hat{S}_{2,x} + \hat{S}_{1,y}\hat{S}_{2,y}). \end{aligned}$$

Method #2: directly use Baker-Hausdorff formula,

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

use the result of Homework #1 Problem 5, $\exp[-\mathbf{i}\theta \cdot (\hat{S}_{1,z} - \hat{S}_{2,z})] \cdot \hat{\chi}_z \cdot \exp[\mathbf{i}\theta \cdot (\hat{S}_{1,z} - \hat{S}_{2,z})]$
 $= \exp(2\theta\hat{A})\hat{B}\exp(-2\theta\hat{A}) = \hat{B}\cos(2\theta) + \hat{C}\sin(2\theta)$
 $= \cos(2\theta)\hat{\chi}_z + \sin(2\theta)(\hat{S}_{1,x}\hat{S}_{2,x} + \hat{S}_{1,y}\hat{S}_{2,y})$.

(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 $\hat{\chi}_z = \frac{1}{2}(\mathbf{i}\hat{S}_{1,+}\hat{S}_{2,-} - \mathbf{i}\hat{S}_{1,-}\hat{S}_{2,+})$, and $\hat{S}_{i,+}|S_{i,z} = 0\rangle = \sqrt{2}|S_{i,z} = 1\rangle, \dots$

$S_{1+2,z}$	\hat{H} in subspace	2nd order ground state energy
2	$(-J) + (0)$	$-J$
1	$\begin{pmatrix} -J & 0 \\ 0 & J \end{pmatrix} + \begin{pmatrix} 0 & -\mathbf{i}D \\ \mathbf{i}D & 0 \end{pmatrix}$	$\approx -J + \frac{(-\mathbf{i}D) \cdot (\mathbf{i}D)}{-J-J} = -J - \frac{D^2}{2J}$
0	$\begin{pmatrix} -J & 0 & 0 \\ 0 & J & 0 \\ 0 & 0 & 2J \end{pmatrix} + \begin{pmatrix} 0 & -\frac{2\mathbf{i}}{\sqrt{3}}D & 0 \\ \frac{2\mathbf{i}}{\sqrt{3}}D & 0 & -\sqrt{\frac{2}{3}}\mathbf{i}D \\ 0 & \sqrt{\frac{2}{3}}\mathbf{i}D & 0 \end{pmatrix}$	$\approx -J + \frac{(-2\mathbf{i}D/\sqrt{3}) \cdot (2\mathbf{i}D/\sqrt{3})}{-J-J} = -J - \frac{2D^2}{3J}$
-1	$\begin{pmatrix} -J & 0 \\ 0 & J \end{pmatrix} + \begin{pmatrix} 0 & -\mathbf{i}D \\ \mathbf{i}D & 0 \end{pmatrix}$	$\approx -J + \frac{(-\mathbf{i}D) \cdot (\mathbf{i}D)}{-J-J} = -J - \frac{D^2}{2J}$
-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 $\hat{U} = e^{-i\theta(\hat{S}_{1,z} - \hat{S}_{2,z})}$ with appropriate θ , we can get $\hat{U}\hat{H}\hat{U}^\dagger$
 $= -J\hat{S}_{1,z}\hat{S}_{2,z} - \sqrt{J^2 + D^2}(\hat{S}_{1,x}\hat{S}_{2,x} + \hat{S}_{1,y}\hat{S}_{2,y}) = -\sqrt{J^2 + D^2}\hat{\mathbf{J}}_1 \cdot \hat{\mathbf{J}}_2 + (\sqrt{J^2 + D^2} - J)\hat{S}_{1,z}\hat{S}_{2,z}.$
 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,
 $\hat{V}_I(t) \equiv e^{i\hat{H}_0 t/\hbar} \cdot (D\hat{\chi}_z) \cdot e^{-i\hat{H}_0 t/\hbar}$. Then the interaction picture time evolution operator is
 $\hat{U}_I(t) \equiv e^{i\hat{H}_0 t/\hbar} e^{-i\hat{H} t/\hbar} = \mathbb{1} + \frac{-i}{\hbar} \int_0^t dt_1 \hat{V}_I(t_1) + (\frac{-i}{\hbar})^2 \int_0^t dt_1 \int_0^{t_1} dt_2 \hat{V}_I(t_1) \hat{V}_I(t_2) + \dots$

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 $\begin{pmatrix} 0 & -\frac{2i}{\sqrt{3}}D \cdot e^{-i2J/\hbar t} & 0 \\ \frac{2i}{\sqrt{3}}D \cdot e^{i2J/\hbar t} & 0 & -\sqrt{\frac{2}{3}}iD \cdot e^{-iJ/\hbar t} \\ 0 & \sqrt{\frac{2}{3}}iD \cdot e^{iJ/\hbar t} & 0 \end{pmatrix}$, $|\psi(t=0)\rangle$ is $\begin{pmatrix} \frac{1}{\sqrt{6}} \\ \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{3}} \end{pmatrix}$. Then
 $\langle S_{1+2} = 2, S_{1+2,z} = 0 | \hat{U}_I | \psi(t=0) \rangle \approx \frac{1}{\sqrt{6}} + \frac{-i}{\hbar} \int_0^t dt_1 [-\frac{2i}{\sqrt{3}}D \cdot e^{-i2J/\hbar t_1} \cdot \frac{1}{\sqrt{2}}]$
 $+ (\frac{-i}{\hbar})^2 \int_0^t dt_1 \int_0^{t_1} dt_2 [\frac{-2i}{\sqrt{3}}D e^{-i2J/\hbar t_1}] [\frac{2i}{\sqrt{3}}D e^{i2J/\hbar t_2} \cdot \frac{1}{\sqrt{6}} + \frac{-\sqrt{2}i}{\sqrt{3}}D e^{-iJ/\hbar t_2} \cdot \frac{1}{\sqrt{3}}] + \dots$
 $\approx \frac{1}{\sqrt{6}} - \frac{iD}{\sqrt{6}J} (e^{-i2Jt/\hbar} - 1) + \frac{-i}{\hbar} \int_0^t dt_1 [\frac{-2i}{\sqrt{3}}D e^{-i2J/\hbar t_1}] [\frac{-iD}{3\sqrt{2}J} (e^{i2Jt_1/\hbar} - 1) + \frac{-i\sqrt{2}D}{3J} (e^{-iJt_1/\hbar} - 1)]$
 $\approx \frac{1}{\sqrt{6}} - \frac{iD}{\sqrt{6}J} (e^{-i2Jt/\hbar} - 1) + \frac{-i}{\hbar} \int_0^t dt_1 [\frac{-2i}{\sqrt{3}}D e^{-i2J/\hbar t_1}] [\frac{-iD}{3\sqrt{2}J} e^{i2Jt_1/\hbar} + \frac{i\sqrt{2}D}{2J} + \frac{-i\sqrt{2}D}{3J} e^{-iJt_1/\hbar}]$

$$\approx \frac{1}{\sqrt{6}} - \frac{iD}{\sqrt{6}J}(e^{-i2Jt/\hbar} - 1) + \frac{i2D^2}{3\sqrt{6}\hbar J}t + \frac{\sqrt{2}D^2}{2\sqrt{3}J^2}(e^{-i2Jt/\hbar} - 1) - \frac{2\sqrt{2}D^2}{9\sqrt{3}J^2}(e^{-i3Jt/\hbar} - 1).$$

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,

$$\begin{aligned} P_0(|\psi(t)\rangle) &\approx \left[\frac{1}{\sqrt{6}} - \frac{D}{\sqrt{6}J} \sin\left(\frac{2Jt}{\hbar}\right) + \frac{\sqrt{2}D^2}{2\sqrt{3}J^2}(\cos\left(\frac{2Jt}{\hbar}\right) - 1) - \frac{2\sqrt{2}D^2}{9\sqrt{3}J^2}(\cos\left(\frac{3Jt}{\hbar}\right) - 1) \right]^2 + \left[\frac{D}{\sqrt{6}J}(\cos\left(\frac{2Jt}{\hbar}\right) - 1) \right]^2 \\ &\approx \frac{1}{6} - \frac{D}{3J} \sin\left(\frac{2Jt}{\hbar}\right) + \frac{D^2}{J^2} \left[\frac{1}{6} \sin^2\left(\frac{2Jt}{\hbar}\right) + \frac{1}{3}(\cos\left(\frac{2Jt}{\hbar}\right) - 1) - \frac{4}{27}(\cos\left(\frac{3Jt}{\hbar}\right) - 1) + \frac{1}{6}(\cos\left(\frac{2Jt}{\hbar}\right) - 1)^2 \right] \\ &\approx \frac{1}{6} - \frac{D}{3J} \sin\left(\frac{2Jt}{\hbar}\right) - \frac{4D^2}{27J^2}(\cos\left(\frac{3Jt}{\hbar}\right) - 1). \end{aligned}$$

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 $[\hat{S}_{i,a}, \hat{S}_{j,b}] = \delta_{ij} \sum_c i\epsilon_{abc} \hat{S}_{i,c}$ for $i, j = 1, 2, 3$ and $a, b, c = x, y, z$, and $(\hat{S}_i)^2 = \frac{1}{2} \cdot (\frac{1}{2} + 1) = \frac{3}{4}$. A complete orthonormal basis $|\psi_i\rangle$ ($i = 1, \dots, 8$) 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 $C_3 : \hat{S}_1 \mapsto \hat{S}_2, \hat{S}_2 \mapsto \hat{S}_3, \hat{S}_3 \mapsto \hat{S}_1$; and $\sigma : \hat{S}_1 \mapsto \hat{S}_1, \hat{S}_2 \mapsto \hat{S}_3, \hat{S}_3 \mapsto \hat{S}_2$. 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 $\hat{\mathbf{S}}_1 \cdot \hat{\mathbf{S}}_2 + \hat{\mathbf{S}}_2 \cdot \hat{\mathbf{S}}_3 + \hat{\mathbf{S}}_3 \cdot \hat{\mathbf{S}}_1 = \frac{1}{2}(\hat{\mathbf{S}}_1 + \hat{\mathbf{S}}_2 + \hat{\mathbf{S}}_3)^2 + \text{constant}$]

(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 $\hat{\mathbf{S}}^2 \equiv (\sum_{i=1}^3 \hat{\mathbf{S}}_i)^2$ 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 $\sum_{i=1}^3 \hat{\mathbf{S}}_i$	$\frac{3}{2}$	$\frac{3}{2}$	$\frac{1}{2}$
basis state(s)	$ \uparrow\uparrow\uparrow\rangle$	$\frac{1}{\sqrt{3}}(\downarrow\uparrow\uparrow\rangle + \uparrow\downarrow\uparrow\rangle + \uparrow\uparrow\downarrow\rangle)$	$\begin{cases} \frac{1}{\sqrt{6}}(2 \downarrow\uparrow\uparrow\rangle - \uparrow\downarrow\uparrow\rangle - \uparrow\uparrow\downarrow\rangle) \\ \frac{1}{\sqrt{2}}(\uparrow\downarrow\uparrow\rangle - \uparrow\uparrow\downarrow\rangle) \end{cases}$

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

(c) Method #1:

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

$$= \frac{1}{2} \hat{\mathbf{S}}_{1+2+3}^2 - \frac{1}{2} \hat{S}_{1+2+3,z}^2 - \frac{3}{4}.$$

Here $\hat{\mathbf{S}}_{1+2+3} = \hat{\mathbf{S}}_1 + \hat{\mathbf{S}}_2 + \hat{\mathbf{S}}_3$ 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 $\frac{1}{\sqrt{3}} \begin{pmatrix} 1 \\ e^{2\pi i/3} \\ e^{-2\pi i/3} \end{pmatrix}$ and $\frac{1}{\sqrt{3}} \begin{pmatrix} 1 \\ e^{-2\pi i/3} \\ e^{2\pi i/3} \end{pmatrix}$.

(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 $\hat{T}^2 = -\mathbb{1}$), so there must be Kramers degeneracy, all energy levels are at least 2-fold degenerate.

Answer #2: consider $\hat{U} = \exp(-i\pi\hat{S}_{1+2+3,y})$, 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 matrices, $(\Gamma_i)^\dagger = \Gamma_i$, $\text{Tr}(\Gamma_i) = 0$. 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 $U_1 = i\Gamma_1\Gamma_2$, $U_2 = i\Gamma_3\Gamma_4$. 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 $\hat{S}_{1,y} = i[\hat{S}_{1,x}, \hat{S}_{1,z}] = \frac{i}{2}\Gamma_2\Gamma_1$, $\hat{S}_{2,y} = i[\hat{S}_{2,x}, \hat{S}_{2,z}] = \frac{i}{2}\Gamma_4\Gamma_3$. 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 $(2a_2, 0, 2a_1) \cdot \hat{\mathbf{S}}_1 + (2a_4, 0, 2a_3) \cdot \hat{\mathbf{S}}_2$, 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 $|\psi_i\rangle$ ($i = 1, \dots, 8$) 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);

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

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

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

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 $\hat{V} = \hat{V}_{+1} + \hat{V}_{-1}$, $(\hat{V}_{\pm 1})^\dagger = \hat{V}_{\mp 1}$, $[\hat{H}_0, \hat{V}_{\pm 1}] = \pm E_0 \cdot \hat{V}_{\pm 1}$. The perturbation contains only “off-diagonal” terms.

Define unitary operator $e^{\hat{S}}$ with $\hat{S} = \frac{\hat{V}_{+1} - \hat{V}_{-1}}{E_0}$. Then $[\hat{S}, \hat{H}_0] = -\hat{V}$.

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

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

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

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

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

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, $e^{\hat{S}}|n_1, n_2, n_3\rangle$, 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, $\begin{pmatrix} 0 & & & \\ & 0 & & \\ & & E_0 & \\ & & & 0 \end{pmatrix} + \begin{pmatrix} 0 & t & 0 & 0 \\ t & 0 & -t & -t \\ 0 & -t & 0 & 0 \\ 0 & -t & 0 & 0 \end{pmatrix}$, are solved as follows.

Method #1.1: directly use degenerate perturbation theory,

For the first two degenerate levels of \hat{H}_0 , define $\hat{P} = \begin{pmatrix} 1 & & \\ & 1 & \\ & & 0 \\ & & & 0 \end{pmatrix}$, $\hat{Q} = \mathbb{1}_{4 \times 4} - \hat{P}$,

$$\hat{G} = \begin{pmatrix} 0 & & & \\ & 0 & & \\ & \frac{1}{E-E_0} & & \\ & & \frac{1}{E+E_0} & \end{pmatrix}, \text{ the secular equation up to 3rd order is } \hat{P}\hat{V}\hat{P} + \hat{P}\hat{V}\hat{G}\hat{V}\hat{P} + \hat{P}\hat{V}\hat{G}\hat{V}\hat{G}\hat{V}\hat{P}$$

$$= \begin{pmatrix} 0, & t \\ t, & \frac{t^2}{E-E_0} + \frac{t^2}{E+E_0} \end{pmatrix} = \begin{pmatrix} 0, & t \\ t, & \frac{2Et^2}{E^2-E_0^2} \end{pmatrix}. \text{ This is } \frac{Et^2}{E^2-E_0^2}\sigma_0 - \frac{Et^2}{E^2-E_0^2}\sigma_3 + t\sigma_1.$$

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 $\hat{\tilde{H}}_0 = \begin{pmatrix} t & & & \\ & -t & & \\ & & E_0 & \\ & & & -E_0 \end{pmatrix}$, and $\hat{V}' = \begin{pmatrix} 0 & 0 & -\frac{t}{\sqrt{2}} & -\frac{t}{\sqrt{2}} \\ 0 & 0 & \frac{t}{\sqrt{2}} & \frac{t}{\sqrt{2}} \\ -\frac{t}{\sqrt{2}} & \frac{t}{\sqrt{2}} & 0 & 0 \\ -\frac{t}{\sqrt{2}} & \frac{t}{\sqrt{2}} & 0 & 0 \end{pmatrix}$. $\hat{H}' = \hat{\tilde{H}}_0 + \hat{V}'$. We

can now use non-degenerate perturbation theory. Because sign of \hat{V}' can be changed by unitary operator $\begin{pmatrix} 1 & & & \\ & 1 & & \\ & & -1 & \\ & & & -1 \end{pmatrix}$, while maintaining $\hat{\tilde{H}}_0$, so \hat{V}' will only generate even-order perturbations. Up to 3rd order the approximate eigenvalues are

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

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),

$e^{\hat{S}}$ with $\hat{S} = \frac{\hat{V}_{+1} - \hat{V}_{-1}}{E_0}$, $[\hat{S}, \hat{H}_0] = -\hat{V}_{+1} - \hat{V}_{-1}$.

$e^{\hat{S}}(\hat{H}_0 + \hat{V}')e^{-\hat{S}} = e^{\hat{S}}(\hat{H}_0 + \hat{V})e^{-\hat{S}} + e^{\hat{S}}\hat{V}_0e^{-\hat{S}}$, the first term has been computed in (a)

up to $O(t^3)$, $e^{\hat{S}}(\hat{H}_0 + \hat{V})e^{-\hat{S}} = (E_0 + \frac{t^2}{E_0})(\hat{n}_1 - \hat{n}_3) + O(t^4)$.

$e^{\hat{S}}\hat{V}_0e^{-\hat{S}}$ up to $O(t^3)$ is $\hat{V}_0 + [\hat{S}, \hat{V}_0] + \frac{1}{2}[\hat{S}, [\hat{S}, \hat{V}_0]] + O(t^4)$.

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

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

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
$$\begin{pmatrix} 0 & (t - \frac{t^3}{E_0^2}) \\ (t - \frac{t^3}{E_0^2}) & 0 \\ & & E_0 + \frac{t^2}{E_0} \\ & & & -E_0 - \frac{t^2}{E_0} \end{pmatrix}.$$
 Further diag-

onalize 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) 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 $\hat{H}'\hat{U}|\hat{H}' = E, \hat{P} = \lambda\rangle = \hat{U}\hat{H}'\hat{U}^\dagger\hat{U}|\hat{H}' = E, \hat{P} = \lambda\rangle = \hat{U}\hat{H}'|\hat{H}' = E, \hat{P} = \lambda\rangle$

$$= E \cdot \hat{U}|\hat{H}' = E, \hat{P} = \lambda\rangle, \text{ and } \hat{P}\hat{U}|\hat{H}' = E, \hat{P} = \lambda\rangle = -\hat{U}\hat{P}\hat{U}^\dagger\hat{U}|\hat{H}' = E, \hat{P} = \lambda\rangle \\ = -\hat{U}\hat{P}|\hat{H}' = E, \hat{P} = \lambda\rangle = -\lambda \cdot \hat{U}|\hat{H}' = E, \hat{P} = \lambda\rangle.$$

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

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

\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),

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