# Homework #8:
# Brief solutions

1. (20points) This problem is based on Problem 4 of Homework #3. Let the unperturbed Hamiltonian be the "second quantized" Hamiltonian for identical non-interacting particles in 1D harmonic potential, $\hat{H}_0 = \int \mathrm{d}x\, \widehat{\psi(x)}^\dagger \cdot (-\frac{\hbar^2\partial_x^2}{2m} + \frac{m\omega^2 x^2}{2}) \cdot \widehat{\psi(x)} = \sum_{n=0}^{\infty} E_{n,\text{1-body}} \widehat{\psi}_n^\dagger \widehat{\psi}_n$. Here $E_{n,\text{1-body}} = \hbar\omega \cdot (n+\frac{1}{2})$ is the single-particle eigenvalue, $\widehat{\psi}_n^\dagger$ is the creation operator for the $n$th single-particle eigenstate of harmonic oscillator, $\widehat{\psi(x)}^\dagger$ is the creation operator for the position basis $|x\rangle$. Let the perturbation term be the "second quantized" 2-body interaction, $\hat{V} = \frac{1}{2}\int \mathrm{d}x \int \mathrm{d}x'\, \widehat{\psi(x)}^\dagger \widehat{\psi(x')}^\dagger \cdot (x-x')^2 \cdot \widehat{\psi(x')}\widehat{\psi(x)}$. You can use the result of Problem 4(c) of Homework #3 to rewrite $\hat{V}$ in terms of $\widehat{\psi}_n^\dagger$ and $\widehat{\psi}_n$. The full Hamiltonian is $\hat{H} = \hat{H}_0 + \lambda\hat{V}$, where $\lambda$ is a small real parameter.

(a) (7pts) *For $N$ identical bosons, solve the ground state energy of $\hat{H}$ up to $\lambda^2$ order by perturbation theory.* Here integer $N \geq 2$.

(b) (7pts) *For $N$ identical fermions, solve the ground state energy of $\hat{H}$ up to $\lambda^2$ order by perturbation theory.* Here integer $N \geq 2$.

(c) (6pts)(*) When particle number $N=2$, eigenvalues and eigenstates of $\hat{H}$ can be solved exactly. Use the "first quantized" form, $\hat{H} = -\frac{\hbar^2}{2m}[(\frac{\partial}{\partial x_1})^2 + (\frac{\partial}{\partial x_2})^2] + \frac{m\omega^2}{2}(x_1^2+x_2^2) + \lambda\,(x_1-x_2)^2$. Then $\hat{H}\psi(x_1,x_2) = E\,\psi(x_1,x_2)$ can be solved by changing variables to the "center of mass" position $x_{\text{COM}} \equiv \frac{x_1+x_2}{2}$ and the relative position $X \equiv x_1 - x_2$. *Solve the exact ground state energy for two-boson and two-fermion cases respectively. Compare with the results of (a)(b) for $N=2$.* [Note: $\psi(x_1,x_2)$ has different symmetry for boson and fermion cases.]

**Solution**:

Use the result of Problem 4(c) of Homework #3,

$$\hat{V} = \frac{\hbar}{4m\omega}\sum_{n,m=0}^{\infty}\Big[ 2\sqrt{(n+2)(n+1)}\widehat{\psi_n}^\dagger\widehat{\psi_m}^\dagger\widehat{\psi_m}\widehat{\psi_{n+2}} - 2\sqrt{(m+1)(n+1)}\widehat{\psi_n}^\dagger\widehat{\psi_m}^\dagger\widehat{\psi_{m+1}}\widehat{\psi_{n+1}}$$
$$+2\sqrt{(n+2)(n+1)}\widehat{\psi_{n+2}}^\dagger\widehat{\psi_m}^\dagger\widehat{\psi_m}\widehat{\psi_n} - 2\sqrt{(m+1)(n+1)}\widehat{\psi_{n+1}}^\dagger\widehat{\psi_{m+1}}^\dagger\widehat{\psi_m}\widehat{\psi_n}$$
$$+2(2n+1)\widehat{\psi_n}^\dagger\widehat{\psi_m}^\dagger\widehat{\psi_m}\widehat{\psi_n} - 2\sqrt{(m+1)(n+1)}(\widehat{\psi_n}^\dagger\widehat{\psi_{m+1}}^\dagger\widehat{\psi_m}\widehat{\psi_{n+1}} + \widehat{\psi_{n+1}}^\dagger\widehat{\psi_m}^\dagger\widehat{\psi_{m+1}}\widehat{\psi_n})\Big].$$

Note that the terms in 1st line decrease $\hat{H}_0$ eigenvalue by $2\hbar\omega$, the terms in 2nd line increase $\hat{H}_0$ eigenvalue by $2\hbar\omega$, the terms in last line do not change $\hat{H}_0$ eigenvalue.

(a). The unperturbed ground state of $\hat{H}_0$ for $N$ bosons is the $N$-fold occupied single-particle ground state, $|\psi_0^{(0)}\rangle \equiv \frac{1}{\sqrt{N!}}(\widehat{\psi}_0^\dagger)^N|\text{vac}\rangle$, with energy $E_0^{(0)} = N \cdot E_{0,\text{1-body}} = \frac{N}{2}\hbar\omega$.

$\hat{V}|\psi_0^{(0)}\rangle = \frac{\hbar}{4m\omega}\Big[0 - 0$
$+2\sqrt{2} \cdot \frac{1}{\sqrt{N!}} \cdot N(N-1) \cdot \widehat{\psi}_2^\dagger(\widehat{\psi}_0^\dagger)^{N-1}$ {note: n=m=0}
$-2 \cdot \frac{1}{\sqrt{N!}} \cdot N(N-1) \cdot (\widehat{\psi}_1^\dagger)^2(\widehat{\psi}_0^\dagger)^{N-2}$ {note: n=m=0}
$+2 \cdot \frac{1}{\sqrt{N!}} \cdot N(N-1) \cdot (\widehat{\psi}_0^\dagger)^N$ {note: n=m=0}
$-0 - 0\Big]|\text{vac}\rangle$
$= \frac{\hbar}{4m\omega}\Big[2N(N-1)|\psi_0^{(0)}\rangle + 2\sqrt{2N}(N-1)|\psi_{2,1}^{(0)}\rangle - 2\sqrt{2N(N-1)}|\psi_{2,2}^{(0)}\rangle\Big].$

Here $|\psi_{2,1}^{(0)}\rangle \equiv \frac{1}{\sqrt{(N-1!}}\widehat{\psi}_2^\dagger(\widehat{\psi}_0^\dagger)^{N-1}|\text{vac}\rangle$, $|\psi_{2,2}^{(0)}\rangle \equiv \frac{1}{\sqrt{2!(N-2)!}}(\widehat{\psi}_1^\dagger)^2(\widehat{\psi}_0^\dagger)^{N-2}|\text{vac}\rangle$ are degenerate 2nd excited states of $\hat{H}_0$ with eigenvalue $E_2^{(0)} = E_0^{(0)} + 2\hbar\omega$.

The ground state energy of $\hat{H}$ upto $\lambda^2$ order is

$E_0 \approx \frac{N}{2}\hbar\omega + \lambda \cdot \frac{\hbar}{4m\omega} \cdot 2N(N-1) + \lambda^2 \cdot (\frac{\hbar}{4m\omega})^2 \frac{|2\sqrt{2N}(N-1)|^2+|-2\sqrt{2N(N-1)}|^2}{-2\hbar\omega}$
$= \frac{N}{2}\hbar\omega + \frac{\lambda\hbar N(N-1)}{2m\omega} - \frac{\lambda^2\hbar N^2(N-1)}{4m^2\omega^3}.$

(b) The unperturbed ground state of $\hat{H}_0$ for $N$ fermion is, $|\psi_0^{(0)}\rangle \equiv (\prod_{i=0}^{N-1}\widehat{\psi}_i^\dagger)|\text{vac}\rangle$, with energy $E_0^{(0)} = \sum_{i=0}^{N-1} E_{i,\text{1-body}} = \frac{N^2}{2}\hbar\omega$.

$\hat{V}|\psi_0^{(0)}\rangle = \frac{\hbar}{4m\omega}\Big[0 - 0$
$+(2\sqrt{(N+1)N}(N-1)(\prod_{i=0}^{N-2}\widehat{\psi}_i^\dagger)\widehat{\psi}_{N+1}^\dagger$ {note: n=N-1; m=1,...,N-2}
$+2\sqrt{N(N-1)}(N-1)(\prod_{i=1}^{N-3}\widehat{\psi}_i^\dagger)\widehat{\psi}_N^\dagger\widehat{\psi}_{N-1}^\dagger)$ {note: n=N-2; m=1,...,N-3,N-1}
$-2 \cdot 2\sqrt{N(N-1)}(\prod_{i=1}^{N-3}\widehat{\psi}_i^\dagger)\widehat{\psi}_{N-1}^\dagger\widehat{\psi}_N^\dagger$ {note: n=N-1; m=N-2; or n=N-2; m=N-1}
$+(N-1)(\sum_{n=0}^{N-1} 2(2n+1))(\prod_{i=1}^{N-1}\widehat{\psi}_i^\dagger)$ {note: n,m=1,...,N-1, and n $\neq$ m}
$+(\sum_{n=0}^{N-2} 2(n+1))(\prod_{i=1}^{N-1}\widehat{\psi}_i^\dagger)$ {note: n=m=1,...,N-2}
$+(\sum_{n=0}^{N-2} 2(n+1))(\prod_{i=1}^{N-1}\widehat{\psi}_i^\dagger)$ {note: n=m=1,...,N-2}$\Big]|\text{vac}\rangle$
$= \frac{\hbar}{4m\omega}\Big[2(N+1)N(N-1)|\psi_0^{(0)}\rangle + 2\sqrt{N(N+1)}(N-1)|\psi_{2,1}^{(0)}\rangle - 2\sqrt{N(N-1)}(N+1)|\psi_{2,2}^{(0)}\rangle\Big].$

Here $|\psi_{2,1}^{(0)}\rangle \equiv (\prod_{i=0}^{N-2}\widehat{\psi}_i^\dagger)\widehat{\psi}_{N+1}^\dagger|\text{vac}\rangle$, $|\psi_{2,2}^{(0)}\rangle \equiv (\prod_{i=1}^{N-3}\widehat{\psi}_i^\dagger)\widehat{\psi}_{N-1}^\dagger\widehat{\psi}_N^\dagger|\text{vac}\rangle$ are degenerate 2nd excited states of $\hat{H}_0$ with eigenvalue $E_2^{(0)} = E_0^{(0)} + 2\hbar\omega$.

The ground state energy of $\hat{H}$ upto $\lambda^2$ order is

$E_0 \approx \frac{N^2}{2}\hbar\omega + \lambda \cdot \frac{\hbar}{4m\omega} \cdot 2(N+1)N(N-1) + \lambda^2 \cdot (\frac{\hbar}{4m\omega})^2 \frac{|2\sqrt{N(N+1)}(N-1)|^2+|-2\sqrt{N(N-1)}(N+1)|^2}{-2\hbar\omega}$
$= \frac{N^2}{2}\hbar\omega + \frac{\lambda\hbar(N+1)N(N-1)}{2m\omega} - \frac{\lambda^2\hbar(N+1)N^2(N-1)}{4m^2\omega^3}.$

(c) Define $\hat{p}_{\text{COM}} = -\mathrm{i}\hbar\partial_{x_{\text{COM}}} = \hat{p}_1 + \hat{p}_2$ and $\hat{P} \equiv -\mathrm{i}\hbar\partial_X = \frac{\hat{p}_1 - \hat{p}_2}{2}$, then $[\hat{x}_{\text{COM}}, \hat{p}_{\text{COM}}] = \mathrm{i}\hbar$,

$[\hat{x}_{\text{COM}}, \hat{P}] = 0$, $[\hat{X}, \hat{p}_{\text{COM}}] = 0$, $[\hat{X}, \hat{P}] = \mathbb{i}\hbar$,

The two-body Hamiltonian is $\hat{H} = (\frac{\hat{p}_{\text{COM}}^2}{2(2m)} + \frac{(2m)\omega^2}{2}\hat{x}_{\text{COM}}^2) + (\frac{\hat{P}^2}{2(m/2)} + \frac{(m/2)(\omega^2+\frac{4\lambda}{m})}{2}\hat{X}^2)$.

This looks like two decoupled harmonic oscillators.

Denote the normalized $n$th eigenstate for harmonic oscillator with mass $m$ and frequency $\omega$ by $\psi_n^{(m,\omega)}(x)$.

For bosons $\psi(x_1, x_2) = \psi(x_2, x_1)$, so wavefunction for $X$ must be even. The ground state for two bosons is $\psi_0^{(2m,\omega)}(x_{\text{COM}}) \cdot \psi_0^{(m/2,\sqrt{\omega^2+\frac{4\lambda}{m}})}(X)$, with energy
$E_0 = \frac{1}{2}\hbar\omega + \frac{1}{2}\hbar\sqrt{\omega^2 + \frac{4\lambda}{m}} \approx \hbar\omega + \frac{\lambda\hbar}{m\omega} - \frac{\lambda^2\hbar}{m\omega^3}$.

For fermions $\psi(x_1, x_2) = -\psi(x_2, x_1)$, so wavefunction for $X$ must be odd. The ground state for two fermions is $\psi_0^{(2m,\omega)}(x_{\text{COM}}) \cdot \psi_1^{(m/2,\sqrt{\omega^2+\frac{4\lambda}{m}})}(X)$, with energy
$E_0 = \frac{1}{2}\hbar\omega + \frac{3}{2}\hbar\sqrt{\omega^2 + \frac{4\lambda}{m}} \approx 2\hbar\omega + \frac{3\lambda\hbar}{m\omega} - \frac{3\lambda^2\hbar}{m\omega^3}$.

2. (15points) Consider three fermion modes, denote their annihilation operators as $\hat{f}_1$, $\hat{f}_2$, $\hat{f}_3$. They satisfy $\{\hat{f}_i, \hat{f}_j^\dagger\} = \delta_{i,j}$. The unperturbed Hamiltonian is $\hat{H}_0 = E_0 \cdot (\hat{n}_1 + \hat{n}_2) + E_1 \cdot \hat{n}_3$. Here $\hat{n}_i = \hat{f}_i^\dagger \hat{f}_i$ is the occupation number operator, $E_1 > E_0$ are real parameters. The occupation basis $|n_1, n_2, n_3\rangle$ are eigenstates of $\hat{H}_0$ with eigenvalue $E_0 \cdot (n_1 + n_2) + E_1 \cdot n_3$, where $n_{1,2,3} = 0$ or $1$ are eigenvalues of $\hat{n}_{1,2,3}$ respectively.

Add a time-independent perturbation, $\hat{V} = -t \cdot (\hat{f}_1^\dagger \hat{f}_2 + \hat{f}_2^\dagger \hat{f}_1 + \hat{f}_1^\dagger \hat{f}_3 + \hat{f}_3^\dagger \hat{f}_1 - \hat{f}_2^\dagger \hat{f}_3 - \hat{f}_3^\dagger \hat{f}_2)$. Here $t$ is a real "small parameter". The perturbed Hamiltonian is $\hat{H} = \hat{H}_0 + \hat{V}$.

(a) (9pts) *Use one of the two approaches (formal series expansion, or unitary transformations) to compute all the energy eigenvalues of $\hat{H}$ in the 2-particle subspace to 3rd order of small parameter $t$.* [Hint: higher order degenerate perturbation theory can be avoided by changing to eigenbasis of 1st order secular equation; certain symmetry may help]

(b) (6pts) *Exactly diagonalize the Hamiltonian $\hat{H}_0 + \hat{V}$ in the 2-particle subspace, expand the exact energy formula to 3rd order of $t$, compare with the perturbation theory result in (a).*

**Solution:**

Choose the occupation basis for the 2-particle space, $(\hat{f}_1^\dagger \hat{f}_2^\dagger|\text{vac}\rangle, \hat{f}_1^\dagger \hat{f}_3^\dagger|\text{vac}\rangle, \hat{f}_2^\dagger \hat{f}_3^\dagger|\text{vac}\rangle)$. Here $|\text{vac}\rangle$ is the fermion vacuum annihilated by all $\hat{f}_i$. Under this basis, $\hat{H}_0$ is diagonal,

$$\hat{H}_0+\hat{V}=\begin{pmatrix}2E_0 & 0 & 0\\ 0 & E_0+E_1 & 0\\ 0 & 0 & E_0+E_1\end{pmatrix}+t\cdot\begin{pmatrix}0 & 1 & 1\\ 1 & 0 & -1\\ 1 & -1 & 0\end{pmatrix}.$$

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

For the $2E_0$ level, $\hat{P}\equiv\begin{pmatrix}1&0&0\\0&0&0\\0&0&0\end{pmatrix}$, $\hat{Q}\equiv\begin{pmatrix}0&0&0\\0&1&0\\0&0&1\end{pmatrix}$, $\hat{G}=\begin{pmatrix}0&0&0\\0&\frac{1}{E-(E_0+E_1)}&0\\0&0&\frac{1}{E-(E_0+E_1)}\end{pmatrix}$.

$\hat{P}|\psi\rangle\equiv|\psi^{(0)}\rangle=\begin{pmatrix}1\\0\\0\end{pmatrix}$. At cubic order of series expansion,

$$E-2E_0=\langle\psi^{(0)}|\left(\hat{V}+\hat{V}\hat{G}\hat{V}+\hat{V}\hat{G}\hat{V}\hat{G}\hat{V}\right)|\psi^{(0)}\rangle=0+\frac{2t^2}{E-(E_0+E_1)}-\frac{2t^3}{[E-(E_0+E_1)]^2}.$$

Plug in the 1st order approximation $E\approx 2E_0+0\cdot t$, we have

$$E\approx 2E_0+0\cdot t+\frac{2t^2}{(E_0-E_1)}-\frac{2t^3}{(E_0-E_1)^2}.$$

For the degenerate $E_0+E_1$ levels, $\hat{P}\equiv\begin{pmatrix}0&0&0\\0&1&0\\0&0&1\end{pmatrix}$, $\hat{Q}\equiv\begin{pmatrix}1&0&0\\0&0&0\\0&0&0\end{pmatrix}$, $\hat{G}=\begin{pmatrix}\frac{1}{E-2E_0}&0&0\\0&0&0\\0&0&0\end{pmatrix}$.

$\hat{P}|\psi\rangle\equiv|\psi^{(0)}\rangle=\begin{pmatrix}0\\c_1\\c_2\end{pmatrix}$. At cubic order of series expansion, the secular equation is

$$[E-(E_0+E_1)]\cdot\begin{pmatrix}0\\c_1\\c_2\end{pmatrix}=\left[\hat{P}\hat{V}\hat{P}+\hat{P}\hat{V}\hat{G}\hat{V}\hat{P}+\hat{P}\hat{V}\hat{G}\hat{V}\hat{G}\hat{V}\hat{P}\right]\cdot\begin{pmatrix}0\\c_1\\c_2\end{pmatrix}$$

$$=\begin{pmatrix}0&0&0\\0&\frac{t^2}{E-2E_0}&-t+\frac{t^2}{E-2E_0}\\0&-t+\frac{t^2}{E-2E_0}&\frac{t^2}{E-2E_0}\end{pmatrix}\cdot\begin{pmatrix}0\\c_1\\c_2\end{pmatrix}.$$

Fortunately this secular equation can be solved analytically. The formal solution is $E-(E_0+E_1)=\frac{t^2}{E-2E_0}\pm(-t+\frac{t^2}{E-2E_0})$.

For the $+$ sign solution, the 1st order approximation is $E\approx(E_0+E_1)-t$, plug this into the other terms on the right-hand-side, and keep terms up to $t^3$, we have

$$E\approx(E_0+E_1)-t+\frac{2t^2}{(E_0+E_1)-t-2E_0}\approx(E_0+E_1)-t+\frac{2t^2}{E_1-E_0}+\frac{2t^3}{(E_1-E_0)^2}.$$

For the $-$ sign solution, the 1st order approximation is $E \approx (E_0+E_1)+t$, plug this into the other terms on the right-hand-side, and keep terms up to $t^3$, we have $E \approx (E_0+E_1)+t$.

Method #2: use unitary transformation directly,

Let $\hat{V} = \hat{V}_0 + \hat{V}_{+1} + \hat{V}_{-1}$, where $\hat{V}_{+1} = t\cdot(-\hat{f}_3^\dagger \hat{f}_1 + \hat{f}_3^\dagger \hat{f}_2)$, $\hat{V}_{-1} = (\hat{V}_{+1})^\dagger = t\cdot(-\hat{f}_1^\dagger \hat{f}_3 + \hat{f}_2^\dagger \hat{f}_3)$, $\hat{V}_0 = t\cdot(-\hat{f}_1^\dagger \hat{f}_2 - \hat{f}_2^\dagger \hat{f}_1)$. Then $[\hat{V}_m, \hat{H}_0] = -m\cdot(E_1-E_0)\hat{V}_m$, for $m=-1,0,+1$.

Define $\hat{H}^{(1)} = \exp(\mathbb{i}\hat{S})\cdot\hat{H}\cdot\exp(-\mathbb{i}\hat{S})$. Demand that $[\mathbb{i}\hat{S},\hat{H}_0] + \hat{V}_{+1} + \hat{V}_{-1} = 0$, then $\mathbb{i}\hat{S} = \frac{1}{E_1-E_0}(\hat{V}_{+1} - \hat{V}_{-1})$. Expand $\hat{H}^{(1)}$ to 3rd order,
$\hat{H}^{(1)} = \hat{H}_0 + \hat{V}_0 + [\mathbb{i}\hat{S},\hat{V}_0] + (1-\frac{1}{2})[\mathbb{i}\hat{S},\hat{V}_{+1}+\hat{V}_{-1}] + \frac{1}{2}[\mathbb{i}\hat{S},[\mathbb{i}\hat{S},\hat{V}_0]] + (\frac{1}{2}-\frac{1}{6})[\mathbb{i}\hat{S},[\mathbb{i}\hat{S},\hat{V}_{+1}+\hat{V}_{-1}]] + \dots$

Compute the commutators order by order, for this problem using the fact that $[\sum_{i,j}\hat{f}_i^\dagger P_{ij}\hat{f}_j, \sum_{k,\ell}\hat{f}_k^\dagger Q_{k\ell}\hat{f}_\ell] = \sum_{i,\ell}\hat{f}_i^\dagger (P\cdot Q - Q\cdot P)_{i\ell}\hat{f}_\ell$..

$[\mathbb{i}\hat{S},\hat{V}_0] = (\hat{f}_1^\dagger, \hat{f}_2^\dagger, \hat{f}_3^\dagger)\left[\frac{1}{E_1-E_0}\begin{pmatrix} 0 & 0 & t \\ 0 & 0 & -t \\ -t & t & 0\end{pmatrix}, \begin{pmatrix} 0 & -t & 0 \\ -t & 0 & 0 \\ 0 & 0 & 0\end{pmatrix}\right]\begin{pmatrix}\hat{f}_1 \\ \hat{f}_2 \\ \hat{f}_3\end{pmatrix} = \frac{t^2}{E_1-E_0}(-\hat{f}_1^\dagger\hat{f}_3 + \hat{f}_2^\dagger\hat{f}_3 - \hat{f}_3^\dagger\hat{f}_1 + \hat{f}_3^\dagger\hat{f}_2) = \frac{t}{E_1-E_0}\cdot(\hat{V}_{+1}+\hat{V}_{-1})$, off-diagonal, order $t^2$.

$[\mathbb{i}\hat{S},\hat{V}_{+1}+\hat{V}_{-1}] = \frac{2}{E_1-E_0}[\hat{V}_{+1},\hat{V}_{-1}] = \frac{2t^2}{E_1-E_0}(-\hat{n}_1 - \hat{n}_2 + 2\hat{n}_3 + \hat{f}_1^\dagger\hat{f}_2 + \hat{f}_2^\dagger\hat{f}_1)$, diagonal, order $t^2$.

Then $[\mathbb{i}\hat{S},[\mathbb{i}\hat{S},\hat{V}_0]] = [\mathbb{i}\hat{S}, \frac{t}{E_1-E_0}\cdot(\hat{V}_{+1}+\hat{V}_{-1})] = \frac{2t^3}{(E_1-E_0)^2}(-\hat{n}_1 - \hat{n}_2 + 2\hat{n}_3 + \hat{f}_1^\dagger\hat{f}_2 + \hat{f}_2^\dagger\hat{f}_1)$.

$[\mathbb{i}\hat{S},[\mathbb{i}\hat{S},\hat{V}_{+1}+\hat{V}_{-1}]] = \frac{8t^3}{(E_1-E_0)^2}(\hat{f}_1^\dagger\hat{f}_3 - \hat{f}_2^\dagger\hat{f}_3 + \hat{f}_3^\dagger\hat{f}_1 - \hat{f}_3^\dagger\hat{f}_2)$, off-diagonal, order $t^3$.

The off-diagonal terms in $\hat{H}^{(1)}$ are at least of order $t^2$, they can be removed by: $\hat{H}^{(2)} = \exp(\mathbb{i}\hat{S}_1)\cdot\hat{H}^{(1)}\cdot\exp(-\mathbb{i}\hat{S}_1)$, and $[\mathbb{i}\hat{S}_1,\hat{H}_0] + (\text{order } t^2 \text{ off-diagonal terms in } \hat{H}^{(1)}) = 0$. But this will generate corrections to diagonal terms at $t^4$ or higher order.

So up to $t^3$ order, the diagonal terms are $\hat{H}_0 + \hat{V}_0 + \frac{t^2}{E_1-E_0}(-\hat{n}_1 - \hat{n}_2 + 2\hat{n}_3 + \hat{f}_1^\dagger\hat{f}_2 + \hat{f}_2^\dagger\hat{f}_1) + \frac{t^3}{(E_1-E_0)^2}(-\hat{n}_1 - \hat{n}_2 + 2\hat{n}_3 + \hat{f}_1^\dagger\hat{f}_2 + \hat{f}_2^\dagger\hat{f}_1)$. In the 2-particle space, this is $\begin{pmatrix} 2E_0 & 0 & 0 \\ 0 & E_0+E_1 & 0 \\ 0 & 0 & E_0+E_1\end{pmatrix} + (\frac{t^2}{E_1-E_0} + \frac{t^3}{(E_1-E_0)^2})\cdot\begin{pmatrix} -2 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1\end{pmatrix} - (t - \frac{t^2}{E_1-E_0} - \frac{t^3}{(E_1-E_0)^2})\cdot\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0\end{pmatrix}$.

Further diagonalize this matrix (the bottom-right $2\times 2$ block), the eigenvalues are

$2E_0 - \frac{2t^2}{E_1-E_0} - \frac{2t^3}{(E_1-E_0)^2}$,

$$E_0 + E_1 + \frac{t^2}{E_1-E_0} + \frac{t^3}{(E_1-E_0)^2} \mp (t - \frac{t^2}{E_1-E_0} - \frac{t^3}{(E_1-E_0)^2}) = \begin{cases} E_0 + E_1 - t + \frac{2t^2}{E_1-E_0} + \frac{2t^3}{(E_1-E_0)^2}, \\ E_0 + E_1 + t. \end{cases}$$

Method #3: diagonalization by symmetry first.

Consider the following unitary transform, $\sigma: \quad \hat{f}_1 \mapsto -\hat{f}_2,\ \hat{f}_2 \mapsto -\hat{f}_1,\ \hat{f}_3 \mapsto \hat{f}_3$. It is easy to see that $\hat{H}$ is invariant under the action of $\sigma$, and $\sigma^2$ is identity operator.

Change basis to $\hat{f}'_1 = \frac{1}{\sqrt{2}}(\hat{f}_1 + \hat{f}_2)$, $\hat{f}'_2 = \frac{1}{\sqrt{2}}(\hat{f}_1 - \hat{f}_2)$, $\hat{f}'_3 = \hat{f}_3$.

Then the action of symmetry generator $\sigma$ is diagonal, $\sigma: \quad \hat{f}'_{2,3} \mapsto \hat{f}'_{2,3},\ \hat{f}'_1 \mapsto -\hat{f}'_1$.

Under the new basis, $\hat{H} = E_0 \cdot (\hat{n}'_1 + \hat{n}'_2) + E_1 \cdot \hat{n}'_3 + t \cdot (\hat{n}'_2 - \hat{n}'_1 - \sqrt{2}\hat{f}'^{\dagger}_2 \hat{f}'_3 - \sqrt{2}\hat{f}'^{\dagger}_3 \hat{f}'_2)$.

One can then proceed like Method #1 or #2. Under the occupation basis of $\hat{f}'$ fermions, the Hamiltonian in the 2-particle space is $\begin{pmatrix} 2E_0 & 0 & 0 \\ 0 & E_0 + E_1 & 0 \\ 0 & 0 & E_0 + E_1 \end{pmatrix} + t \cdot \begin{pmatrix} 0 & -\sqrt{2} & 0 \\ -\sqrt{2} & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$.

The third basis is decoupled from the others, with exact eigenvalue $E_0 + E_1 + t$. We only need to solve non-degenerate perturbation for the first and second basis.

(b) Use the result of Method #3 above, the exact eigenvalues are

$\frac{3E_0+E_1}{2} - \frac{t}{2} - \frac{1}{2}\sqrt{(E_1 - E_0 - t)^2 + 8t^2} \approx 2E_0 - \frac{2t^2}{E_1 - E_0} - \frac{2t^3}{(E_1-E_0)^2}$,

$\frac{3E_0+E_1}{2} - \frac{t}{2} + \frac{1}{2}\sqrt{(E_1 - E_0 - t)^2 + 8t^2} \approx E_0 + E_1 - t + \frac{2t^2}{E_1 - E_0} + \frac{2t^3}{(E_1-E_0)^2}$,

$E_0 + E_1 + t$.

NOTE: as a consistency check, sum of the three approximate eigenvalues should be equal to the trace of the Hamiltonian, $(2E_0) + (E_0 + E_1) + (E_0 + E_1)$, up to cubic order.

3. (15points) Consider a 2-level system, $\hat{H}_0 = \begin{pmatrix} E_0 & 0 \\ 0 & E_1 \end{pmatrix}$ under basis $(|\psi_0^{(0)}\rangle, |\psi_1^{(0)}\rangle)$ with $E_1 > E_0$. Add a time-dependent perturbation $\hat{V}(t) = V \begin{pmatrix} 0 & e^{-\mathrm{i}\omega t} \\ e^{\mathrm{i}\omega t} & 0 \end{pmatrix}$ under the above basis, where $V > 0$ is a "small parameter", $\omega$ is real. Denote the time-evolution operator in Schrödinger picture of perturbed Hamiltonian $\hat{H}(t) = \hat{H}_0 + \hat{V}(t)$ as $\hat{U}_S(t)$, then $\mathrm{i}\hbar \frac{\mathrm{d}}{\mathrm{d}t}\hat{U}_S(t) = \hat{H}(t) \cdot \hat{U}_S(t)$.

(a) (5pts) *Compute the transition probability* $|\langle\psi_1^{(0}|\hat{U}_S(t)|\psi_0^{(0)}\rangle|^2$ *by perturbative expansion to lowest non-trivial order of* $V$. [Hint: use the interaction picture.]

(b) (5pts) *Compute* $|\langle\psi_0^{(0}|\hat{U}_S(t)|\psi_0^{(0)}\rangle|^2$ *to cubic order of* $V$*.* [Hint: you need to compute $\langle\psi_0^{(0}|\hat{U}_I(t)|\psi_0^{(0)}\rangle$ up to appropriate order of $V$]

(c) (5pts) An exact solution of $|\langle\psi_1^{(0}|\hat{U}_S(t)|\psi_0^{(0)}\rangle|^2$ is possible (Rabi oscillation). *Assume* $|\psi(t)\rangle = c_0(t)e^{-\mathrm{i}E_0t/\hbar}|\psi_0^{(0)}\rangle + c_1(t)e^{-\mathrm{i}E_1t/\hbar}|\psi_0^{(1)}\rangle$ *is the solution of* $\mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t}|\psi(t)\rangle = \hat{H}|\psi(t)\rangle$ *with initial condition* $|\psi(t=0)\rangle = |\psi_0^{(0)}\rangle$*. Derive and solve differential equations for coefficients* $c_0(t)$ *and* $c_1(1)$*.* Then $|\langle\psi_1^{(0}|\hat{U}_S(t)|\psi_0^{(0)}\rangle|^2 = |c_1(t)|^2$. Check that the exact result and approximate result in (a) are consistent for small $V$.

**Solution**:

(a) use the interaction picture, define $\hat{U}_I(t) = e^{\mathrm{i}\hat{H}_0t/\hbar}\hat{U}(t)$, then $\mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t}\hat{U}_I(t) = \hat{V}_I(t)\hat{U}_I(t)$.

Here $\hat{V}_I(t) = e^{\mathrm{i}\hat{H}_0t/\hbar}\hat{V}(t)e^{-\mathrm{i}\hat{H}_0t/\hbar} = V\begin{pmatrix} 0 & e^{-\mathrm{i}(\omega+\frac{E_1-E_0}{\hbar})t} \\ e^{\mathrm{i}(\omega+\frac{E_1-E_0}{\hbar})t} & 0 \end{pmatrix}$.

$|\langle\psi_1^{(0)}|\hat{U}(t)|\psi_0^{(0)}\rangle|^2 = |\langle\psi_1^{(0)}|\hat{U}_I(t)|\psi_0^{(0)}\rangle|^2$, because final state $\langle\psi_1^{(0)}|$ is eigenstate of $\hat{H}_0$.

To lowest order approximation,

$$U_I(t) \approx \mathbb{1} + \frac{-\mathrm{i}}{\hbar}\int_0^t \hat{V}_I(t_1)\,\mathrm{d}t_1 = \begin{pmatrix} 1 & \frac{V}{E_1-E_0+\hbar\omega}(e^{-\mathrm{i}(\omega+\frac{E_1-E_0}{\hbar})t}-1) \\ \frac{-V}{E_1-E_0+\hbar\omega}(e^{\mathrm{i}(\omega+\frac{E_1-E_0}{\hbar})t}-1) & 1 \end{pmatrix}$$

$|\langle\psi_1^{(0)}|\hat{U}_I(t)|\psi_0^{(0)}\rangle|^2 \approx |\frac{-V}{E_1-E_0+\hbar\omega}(e^{\mathrm{i}(\omega+\frac{E_1-E_0}{\hbar})t}-1)|^2$

$= \frac{V^2}{(E_1-E_0+\hbar\omega)^2}\cdot 4\cdot[\sin(\frac{E_1-E_0+\hbar\omega}{2\hbar}t)]^2$ .

(b) $|\langle\psi_0^{(0)}|\hat{U}(t)|\psi_0^{(0)}\rangle|^2 = |\langle\psi_0^{(0)}|\hat{U}_I(t)|\psi_0^{(0)}\rangle|^2$, because final state $\langle\psi_0^{(0)}|$ is eigenstate of $\hat{H}_0$.

We need to keep $\langle\psi_0^{(0)}|\hat{U}_I(t)|\psi_0^{(0)}\rangle$ upto cubic order of $V$, $\langle\psi_0^{(0)}|\hat{U}_I(t)|\psi_0^{(0)}\rangle$

$= 1 + \frac{-\mathrm{i}}{\hbar}\int_0^t \mathrm{d}t_1\,\langle\psi_0^{(0)}|\hat{V}_I(t_1)|\psi_0^{(0)}\rangle + (\frac{-\mathrm{i}}{\hbar})^2\int_0^t \mathrm{d}t_1\int_0^{t_1}\mathrm{d}t_2\,\langle\psi_0^{(0)}|\hat{V}_I(t_1)\hat{V}_I(t_2)|\psi_0^{(0)}\rangle$

$+(\frac{-\mathrm{i}}{\hbar})^3\int_0^t \mathrm{d}t_1\int_0^{t_1}\mathrm{d}t_2\int_0^{t_2}\mathrm{d}t_3\,\langle\psi_0^{(0)}|\hat{V}_I(t_1)\hat{V}_I(t_2)\hat{V}_I(t_3)|\psi_0^{(0)}\rangle + O(V^4)$.

Note that $\langle\psi_0^{(0)}|\hat{V}_I(t_1)|\psi_0^{(0)}\rangle = 0$, $\langle\psi_0^{(0)}|\hat{V}_I(t_1)\hat{V}_I(t_2)\hat{V}_I(t_3)|\psi_0^{(0)}\rangle = 0$,

$\langle\psi_0^{(0)}|\hat{V}_I(t_1)\hat{V}_I(t_2)|\psi_0^{(0)}\rangle = V^2e^{-\mathrm{i}\tilde{\omega}t_1}e^{\mathrm{i}\tilde{\omega}t_2}$. Here for simplicity we define $\tilde{\omega} = \omega + \frac{E_1-E_0}{\hbar}$.

$\langle\psi_0^{(0)}|\hat{U}_I(t)|\psi_0^{(0)}\rangle \approx 1 - \frac{V^2}{\hbar^2}\int_0^t \mathrm{d}t_1\int_0^{t_1}\mathrm{d}t_2\,e^{-\mathrm{i}\tilde{\omega}t_1}e^{\mathrm{i}\tilde{\omega}t_2} = 1 - \frac{V^2}{\hbar^2}\int_0^t \mathrm{d}t_1\,e^{-\mathrm{i}\tilde{\omega}t_1}\frac{e^{\mathrm{i}\tilde{\omega}t_1}-1}{\mathrm{i}\tilde{\omega}}$

$= 1 + \mathrm{i}\frac{V^2}{\hbar^2}\frac{t}{\tilde{\omega}} + \frac{V^2}{\hbar^2}\frac{e^{-\mathrm{i}\tilde{\omega}t}-1}{\tilde{\omega}^2} = (1 - \frac{2V^2}{\hbar^2\tilde{\omega}^2}\sin^2(\frac{\tilde{\omega}t}{2})) + \mathrm{i}\frac{V^2}{\hbar^2}(\frac{t}{\tilde{\omega}} - \frac{1}{\tilde{\omega}^2}\sin(\tilde{\omega}t))$.

So up to $V^3$, $|\langle\psi_0^{(0)}|\hat{U}(t)|\psi_0^{(0)}\rangle|^2 \approx (1 - \frac{2V^2}{\hbar^2\tilde{\omega}^2}\sin^2(\frac{\tilde{\omega}t}{2}))^2 + O(V^4)$

$\approx 1 - 2\cdot\frac{2V^2}{\hbar^2\tilde{\omega}^2}\sin^2(\frac{\tilde{\omega}t}{2}) + O(V^4) \approx 1 - \frac{V^2}{(E_1-E_0+\hbar\omega)^2}\cdot 4\cdot[\sin(\frac{E_1-E_0+\hbar\omega}{2\hbar}t)]^2$.

Note that $|\langle\psi_0^{(0)}|\hat{U}(t)|\psi_0^{(0)}\rangle|^2 + |\langle\psi_1^{(0)}|\hat{U}(t)|\psi_0^{(0)}\rangle|^2 = 1$.

(c) Plug the ansatz for $|\psi(t)\rangle$ into the Schrödinger equation.
$\mathbb{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t}\begin{pmatrix} c_0(t) \\ c_1(t) \end{pmatrix} = V\begin{pmatrix} 0 & e^{-\mathbb{i}\tilde{\omega}t} \\ e^{\mathbb{i}\tilde{\omega}t} & 0 \end{pmatrix}\begin{pmatrix} c_0(t) \\ c_1(t) \end{pmatrix}$.

Define $\tilde{c}_0(t) = e^{\mathbb{i}\tilde{\omega}t}c_0(t)$, then $\mathbb{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t}\begin{pmatrix} \tilde{c}_0(t) \\ c_1(t) \end{pmatrix} = \begin{pmatrix} -\hbar\tilde{\omega} & V \\ V & 0 \end{pmatrix}\begin{pmatrix} \tilde{c}_0(t) \\ c_1(t) \end{pmatrix}$.

Therefore $\begin{pmatrix} \tilde{c}_0(t) \\ c_1(t) \end{pmatrix} = \exp[-\frac{\mathbb{i}}{\hbar}\begin{pmatrix} -\hbar\tilde{\omega} & V \\ V & 0 \end{pmatrix}\cdot t]\cdot\begin{pmatrix} \tilde{c}_0(t=0) \\ c_1(t=0) \end{pmatrix}$.

The matrix $\begin{pmatrix} -\hbar\tilde{\omega} & V \\ V & 0 \end{pmatrix} = -\frac{\hbar\tilde{\omega}}{2}\sigma_0 - \frac{\hbar\tilde{\omega}}{2}\sigma_3 + V\sigma_1 = -\frac{\hbar\tilde{\omega}}{2}\sigma_0 + \sqrt{(\frac{\hbar\tilde{\omega}}{2})^2 + V^2}(\boldsymbol{n}\cdot\boldsymbol{\sigma})$, where $\boldsymbol{n} = \frac{1}{\sqrt{(\frac{\hbar\tilde{\omega}}{2})^2+V^2}}(V, 0, -\frac{\hbar\tilde{\omega}}{2})$ is a unit-length vector. Use the result of Homework #1 Problem 6(b), $\exp(-\mathbb{i}\theta\boldsymbol{n}\cdot\boldsymbol{\sigma}) = \cos\theta\sigma_0 - \mathbb{i}\sin(\theta)\boldsymbol{n}\cdot\boldsymbol{\sigma}$.

Then $\exp[-\frac{\mathbb{i}}{\hbar}\begin{pmatrix} -\hbar\tilde{\omega} & V \\ V & 0 \end{pmatrix}\cdot t] = e^{\mathbb{i}\tilde{\omega}t/2}[\cos(\theta t)\sigma_0 - \mathbb{i}\sin(\theta t)\cdot(\boldsymbol{n}\cdot\boldsymbol{\sigma})]$ where $\theta = \sqrt{(\frac{\tilde{\omega}}{2})^2 + (\frac{V}{\hbar})^2}$.

Further use $\begin{pmatrix} \tilde{c}_0(t=0) \\ c_1(t=0) \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$, then $c_1(t) = e^{\mathbb{i}\tilde{\omega}t/2}(\frac{-\mathbb{i}V}{\sqrt{(\frac{\hbar\tilde{\omega}}{2})^2+V^2}})\sin(\frac{1}{2}\sqrt{\tilde{\omega}^2 + (\frac{2V}{\hbar})^2}\cdot t)$.

The transition probability is
$|c_1(t)|^2 = \frac{4V^2}{(\hbar\tilde{\omega})^2+4V^2}[\sin(\frac{\sqrt{\tilde{\omega}^2+4V^2/\hbar^2}}{2}\cdot t]^2 = \frac{4V^2}{(E_1-E_0+\hbar\omega)^2+4V^2}[\sin(\frac{\sqrt{(\omega+\frac{E_1-E_0}{\hbar})^2+4V^2/\hbar^2}}{2}\cdot t]^2$ .

When $V$ is small, one only needs to keep the $V$ in the numerator of prefactor, the result is the same as the 1st order perturbation theory.