Homework #3:
Brief Solutions

***** (about lecture #2) *****

1. Consider the boson coherent state $|z\rangle \equiv e^{-|z|^2/2} e^{z\,\hat{b}^\dagger}|\text{vac}\rangle$, where z is a complex number, $\hat{b}^\dagger$ is a boson creation operator ($[\hat{b},\hat{b}^\dagger]=1$), $|\text{vac}\rangle$ is the normalized boson vacuum state(so $\hat{b}|\text{vac}\rangle = 0$).

(a). (2pts) *Compute the overlap $\langle z'|z\rangle$, where z' and z are two complex numbers.* [Hint: you can expand $|z\rangle$ into occupation basis states, or use some results of Homework #1]

(b). (3pts) *Prove the resolution of identity in terms of these overcomplete basis, $\mathbb{1} = \int_{x=-\infty}^{\infty}\int_{y=-\infty}^{\infty} |x+\mathrm{i}y\rangle\langle x+\mathrm{i}y|\,\frac{\mathrm{d}x\mathrm{d}y}{\pi}$, where x, y are real numbers.* [Hint: represent $x+\mathrm{i}y$ by $r\,e^{\mathrm{i}\theta}$.]

Solution:

The occupation basis $|n\rangle \equiv \frac{1}{\sqrt{n!}}(\hat{b}^\dagger)^n|\text{vac}\rangle$ form complete orthonormal basis in this Fock space. Represent the coherent state by these basis, $|z\rangle = e^{-|z|^2/2}\sum_{n=0}^{\infty}\frac{z^n}{\sqrt{n!}}|n\rangle$.

(a) $\langle z'|z\rangle = e^{-|z'|^2/2}e^{-|z|^2/2}\sum_{n=0}^{\infty}\frac{(z'^*)^n}{\sqrt{n!}}\frac{z^n}{\sqrt{n!}} = \exp(-|z'|^2/2 - |z|^2/2 + z'^* z)$

Method #2: $\langle z'|z\rangle = e^{-|z'|^2/2-|z|^2/2}\langle\text{vac}|e^{z'^*\hat{b}}e^{z\hat{b}^\dagger}|\text{vac}\rangle$.

Use the result of Homework #1 Problem 4(a), $e^{z'^*\hat{b}}e^{z\hat{b}^\dagger} = e^{z\hat{b}^\dagger}e^{z'^*\hat{b}}e^{z'^*z}$, because $[(z')^*\hat{b}, z\hat{b}^\dagger] = z'^*z$ is a c-number.

$e^{z'^*\hat{b}}|\text{vac}\rangle = \left[1+\sum_{n=1}^{\infty}\frac{(z'^*)^n}{n!}(\hat{b})^n\right]|\text{vac}\rangle = |\text{vac}\rangle$, similarly $\langle\text{vac}|e^{z\hat{b}^\dagger} = \langle\text{vac}|$.

Finally $\langle z'|z\rangle = e^{-|z'|^2/2-|z|^2/2}\langle\text{vac}|e^{z'^*\hat{b}}e^{z\hat{b}^\dagger}|\text{vac}\rangle = e^{-|z'|^2/2-|z|^2/2+z'^*z}\langle\text{vac}|e^{z\hat{b}^\dagger}e^{z'^*\hat{b}}|\text{vac}\rangle$
$= e^{-|z'|^2/2-|z|^2/2+z'^*z}\langle\text{vac}|\text{vac}\rangle = e^{-|z'|^2/2-|z|^2/2+z'^*z}$.

(b) $|x+\mathrm{i}y\rangle\langle x+\mathrm{i}y| = \exp(-|x+\mathrm{i}y|^2)\sum_{n=0}^{\infty}\sum_{m=0}^{\infty}|n\rangle\langle m|\cdot\frac{(x+\mathrm{i}y)^n(x-\mathrm{i}y)^m}{\sqrt{n!m!}}$
$= e^{-r^2}\sum_{n=0}^{\infty}\sum_{m=0}^{\infty}|n\rangle\langle m|\cdot\frac{r^{n+m}e^{\mathrm{i}\theta\cdot(n-m)}}{\sqrt{n!m!}}$,

and $\int_{x=-\infty}^{\infty}\int_{y=-\infty}^{\infty}\exp(-|x+\mathrm{i}y|^2)\frac{(x+\mathrm{i}y)^n(x-\mathrm{i}y)^m}{\sqrt{n!m!}}\frac{\mathrm{d}x\mathrm{d}y}{\pi} = \int_{r=0}^{\infty}\int_{\theta=0}^{2\pi}e^{-r^2}\frac{r^{n+m}e^{\mathrm{i}\theta\cdot(n-m)}}{\sqrt{n!m!}}\frac{r\mathrm{d}r\mathrm{d}\theta}{\pi}$
$= \frac{1}{\pi}\int_{r=0}^{\infty}e^{-r^2}\frac{r^{n+m}}{\sqrt{n!m!}}r\mathrm{d}r\cdot\int_{\theta=0}^{2\pi}e^{\mathrm{i}\theta\cdot(n-m)}\,\mathrm{d}\theta = \frac{1}{\pi}\cdot\frac{1}{2}\frac{1}{\sqrt{n!m!}}\int_{(r^2)=0}^{\infty}e^{-r^2}(r^2)^{(n+m)/2}\,\mathrm{d}(r^2)\cdot 2\pi\delta_{n,m}$
$= \delta_{n,m}\left[\Gamma(\frac{n+m}{2}+1)\frac{1}{\sqrt{n!m!}}\right]_{m=n} = \delta_{n,m}$,

therefore $\int_{x=-\infty}^{\infty}\int_{y=-\infty}^{\infty}|x+\mathrm{i}y\rangle\langle x+\mathrm{i}y|\frac{\mathrm{d}x\mathrm{d}y}{\pi} = \sum_{n=0}^{\infty}\sum_{m=0}^{\infty}\delta_{n,m}|n\rangle\langle m| = \sum_{n=0}^{\infty}|n\rangle\langle n|$, which is the resolution of identity in the complete orthonormal basis.

2. Consider a "boson pairing state" $|\psi_\lambda\rangle \equiv \sqrt{1-|\lambda|^2}\cdot\exp(\lambda\hat{b}_1^\dagger\hat{b}_2^\dagger)|\mathrm{vac}\rangle$. Here $[\hat{b}_i,\hat{b}_j^\dagger]=\delta_{i,j}$, $[\hat{b}_i,\hat{b}_j]=0$, λ is a complex number with $|\lambda|<1$, $|\mathrm{vac}\rangle$ is the normalized boson vacuum state (so $\hat{b}_i|\mathrm{vac}\rangle = 0$).

(a). (2pts) *Compute $\langle\psi_\lambda|\psi_\lambda\rangle$ and show that this state is normalized.*

(b). (3pts) Define "Bogoliubov quasiparticle" annihilation operators, $\hat{\gamma}_1 = u\hat{b}_1 + v\hat{b}_2^\dagger$, $\hat{\gamma}_2 = u\hat{b}_2 + v\hat{b}_1^\dagger$, where $u=(1-|\lambda|^2)^{-1/2}$ and $v=-\lambda\,(1-|\lambda|^2)^{-1/2}$. *Check explicitly that $[\hat{\gamma}_i,\hat{\gamma}_j^\dagger]=\delta_{i,j}$, and $\hat{\gamma}_i|\psi_\lambda\rangle = 0$.*

Solution:

Define complete orthonormal occupation basis, $|n_1,n_2\rangle \equiv \frac{1}{\sqrt{n_1!n_2!}}(\hat{b}_1^\dagger)^{n_1}(\hat{b}_2^\dagger)^{n_2}|\mathrm{vac}\rangle$. Then $\hat{b}_1^\dagger|n_1,n_2\rangle = \sqrt{n_1+1}|n_1{+}1,n_2\rangle$, $\hat{b}_2^\dagger|n_1,n_2\rangle = \sqrt{n_2+1}|n_1,n_2{+}1\rangle$, $\hat{b}_1|n_1,n_2\rangle = \sqrt{n_1}|n_1{-}1,n_2\rangle$, $\hat{b}_2|n_1,n_2\rangle = \sqrt{n_2}|n_1,n_2-1\rangle$. Here $n_1,n_2=0,1,\ldots$.

$|\psi_\lambda\rangle = \sqrt{1-|\lambda|^2}\sum_{n=0}^{\infty}\frac{1}{n!}\lambda^n(\hat{b}_1^\dagger\hat{b}_2^\dagger)^n|\mathrm{vac}\rangle = \sqrt{1-|\lambda|^2}\sum_{n=0}^{\infty}\lambda^n|n_1=n,n_2=n\rangle$.

(a) $\langle\psi_\lambda|\psi_\lambda\rangle = |\sqrt{1-|\lambda|^2}|^2\sum_{n=0}^{\infty}(\lambda^*)^n\lambda^n = 1.$

(b) $[\gamma_1,\gamma_1^\dagger] = [u\hat{b}_1+v\hat{b}_2^\dagger, u^*\hat{b}_1^\dagger+v^*\hat{b}_2] = uu^*[\hat{b}_1,\hat{b}_1^\dagger]+0+0+vv^*[\hat{b}_2^\dagger,\hat{b}_2] = |u|^2-|v|^2=1.$ Other commutators are omitted here.

$$\gamma_1|\psi_\lambda\rangle = \sqrt{1-|\lambda|^2}\cdot(\tfrac{1}{\sqrt{1-|\lambda|^2}}\hat{b}_1 - \tfrac{\lambda}{\sqrt{1-|\lambda|^2}}\hat{b}_2^\dagger)\sum_{n=0}^{\infty}\lambda^n|n_1=n,n_2=n\rangle$$
$$= \sqrt{1-|\lambda|^2}\cdot[\tfrac{1}{\sqrt{1-|\lambda|^2}}\sum_{n=0}^{\infty}\lambda^n\sqrt{n}|n_1=n-1,n_2=n\rangle$$
$$- \tfrac{\lambda}{\sqrt{1-|\lambda|^2}}\sum_{n=0}^{\infty}\lambda^n\sqrt{n+1}|n_1=n,n_2=n+1\rangle]$$
$$= \sum_{n=0}^{\infty}\lambda^n\sqrt{n}|n_1=n-1,n_2=n\rangle - \sum_{(n'\equiv n+1)=1}^{\infty}\lambda^{n'}\sqrt{n'}|n_1=n'-1,n_2=n'\rangle = 0.$$

$\gamma_2|\psi_\lambda\rangle$ is similar and omitted here.

3. Consider a single-fermion Hilbert space, with complete orthonormal basis $|e_1\rangle$,$|e_2\rangle$,$|e_3\rangle$. Denote the corresponding creation (annihilation) operators as $\hat{c}_i^\dagger$ ($\hat{c}_i$), for $i=1,2,3$ respec-

tively. Then $\{\hat{c}_i, \hat{c}_j^\dagger\} = \delta_{i,j}$, $\{\hat{c}_i, \hat{c}_j\} = \{\hat{c}_i^\dagger, \hat{c}_j^\dagger\} = 0$, and $|e_i\rangle = \hat{c}_i^\dagger|\text{vac}\rangle$, for $i, j = 1, 2, 3$, where $|\text{vac}\rangle$ is the normalized fermion 'vacuum' state.

(a). (5pts) Define three operators $\hat{S}_x = -\mathbb{i}(\hat{c}_2^\dagger\hat{c}_3 - \hat{c}_3^\dagger\hat{c}_2)$, $\hat{S}_y = -\mathbb{i}(\hat{c}_3^\dagger\hat{c}_1 - \hat{c}_1^\dagger\hat{c}_3)$, $\hat{S}_z = -\mathbb{i}(\hat{c}_1^\dagger\hat{c}_2 - \hat{c}_2^\dagger\hat{c}_1)$. *Compute the commutators,* $[\hat{S}_x, \hat{S}_y]$, $[\hat{S}_y, \hat{S}_z]$, $[\hat{S}_z, \hat{S}_x]$. Represent the results as linear combinations of $\hat{S}_{x,y,z}$. (Hint: check and use the identity $[\hat{A}\hat{B}, \hat{C}\hat{D}] = \hat{A}\{\hat{B}, \hat{C}\}\hat{D} - \{\hat{A}, \hat{C}\}\hat{B}\hat{D} + \hat{C}\hat{A}\{\hat{B}, \hat{D}\} - \hat{C}\{\hat{A}, \hat{D}\}\hat{B}$.)

(b). (5pts) *Write down a complete set of orthonormal basis of the Hilbert space of two fermions.* (Preferably in terms of creation operators) *Compute the matrix elements of* $\hat{S}_{x,y,z}$ *between these bases of two-fermion Hilbert space. Check that these matrix representations of* $\hat{S}_{x,y,z}$ *within the two-fermion Hilbert space do satisfy the commutation relations in (a).* [Hint: be careful about minus signs when computing matrix elements]

(c). (5pts) $\hat{S}_{x,y,z}$ in (a) are all hermitian operators. Then $\exp(\mathbb{i}\theta\hat{S}_x)$ is a unitary operator when θ is a real number. *Compute* $\exp(\mathbb{i}\theta\hat{S}_x) \cdot (a\hat{S}_x + b\hat{S}_y + c\hat{S}_z) \cdot \exp(-\mathbb{i}\theta\hat{S}_x)$ *and represent the result in terms of finite-degree polynomials of* $\hat{S}_{x,y,z}$. Here a, b, c are some complex numbers. [Hint: some results in Homework #1 will be useful]

(d). (5pts) *Solve the eigenvalues of the hermitian operator* $\hat{S}_y - \hat{S}_z$ *in the 8-dimensional Fock space.* [Hint: you can divide the Fock space into subspaces of fixed total fermion number, or try to 'diagonalize' a 'fermion bilinear' operator in similar way as Problem 2(d), some previous results may help]

(e). (5pts) (DIFFICULT) *Solve the eigenvalues and eigenvectors of* $\hat{H} = \hat{c}_1^\dagger\hat{c}_2 + \hat{c}_2^\dagger\hat{c}_1 + \hat{c}_3^\dagger\hat{c}_3 + \hat{c}_3(\hat{c}_1 + \hat{c}_2) + (\hat{c}_1^\dagger + \hat{c}_2^\dagger)\hat{c}_3^\dagger$, *in the 8-dimensional Fock space.* [Hint: use symmetry to divide the Fock space, certain particle-hole transformation and basis change may help]

Solutions:

(a) $[\hat{S}_x, \hat{S}_y] = \mathbb{i}\hat{S}_z$, $[\hat{S}_y, \hat{S}_z] = \mathbb{i}\hat{S}_x$, $[\hat{S}_z, \hat{S}_x] = \mathbb{i}\hat{S}_y$.

Useful fact: for $\hat{P} = \sum_{i,j} \hat{c}_i^\dagger P_{ij}\hat{c}_j$ and $\hat{Q} = \sum_{i,j} \hat{c}_i^\dagger Q_{ij}\hat{c}_j$, the commutator $[\hat{P},\hat{Q}] = [\sum_{i,j} \hat{c}_i^\dagger P_{ij} \hat{c}_j, \sum_{i',j'} \hat{c}_{i'}^\dagger Q_{i'j'} \hat{c}_{j'}] = \sum_{i,j,i',j'} P_{ij} Q_{i'j'} [\hat{c}_i^\dagger \hat{c}_j, \hat{c}_{i'}^\dagger \hat{c}_{j'}]$ $= \sum_{i,j,i',j'} P_{ij} Q_{i'j'} (\hat{c}_i^\dagger \delta_{j,i'} \hat{c}_{j'} - \hat{c}_{i'}^\dagger \delta_{i,j'} \hat{c}_j) = \sum_{i,j} \hat{c}_i^\dagger ([P,Q])_{ij} \hat{c}_j$, where $[P,Q] \equiv (P\cdot Q - Q\cdot P)$ is the commutator of two c-number square matrices P and Q, its matrix element is $([P,Q])_{ij} = \sum_k P_{ik}Q_{kj} - Q_{ik}P_{kj}$.

(b) Note: the choice and ordering of basis are not unique.

Use the occupation basis for the 2-particle space, $|n_1=1,n_2=1,n_3=0\rangle = \hat{c}_1^\dagger \hat{c}_2^\dagger |\text{vac}\rangle$, $|n_1=1,n_2=0,n_3=1\rangle = \hat{c}_1^\dagger \hat{c}_3^\dagger |\text{vac}\rangle$, $|n_1=0,n_2=1,n_3=1\rangle = \hat{c}_2^\dagger \hat{c}_3^\dagger |\text{vac}\rangle$. Then $\hat{S}_x$ is $\begin{pmatrix} 0 & -\mathbb{i} & 0 \\ \mathbb{i} & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$, $\hat{S}_y$ is $\begin{pmatrix} 0 & 0 & -\mathbb{i} \\ 0 & 0 & 0 \\ \mathbb{i} & 0 & 0 \end{pmatrix}$, $\hat{S}_z$ is $\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -\mathbb{i} \\ 0 & \mathbb{i} & 0 \end{pmatrix}$.

It is straightforward to check that these 3×3 matrices satisfy the same commutation relations in (a).

(c) This is exactly the same as Homework #1 Problem 5, by replacing $\hat{A},\hat{B},\hat{C}$ there with $\hat{S}_x,\hat{S}_y,\hat{S}_z$. $\exp(\mathbb{i}\theta\hat{S}_x)\cdot(a\hat{S}_x + b\hat{S}_y + c\hat{S}_z)\cdot\exp(-\mathbb{i}\theta\hat{S}_x) = a\hat{S}_x + (b\cos(\theta)+c\sin(\theta))\hat{S}_y + (-b\sin(\theta)+c\cos(\theta))\hat{S}_z$.

(d) Method #1: brute-force diagonalization.

Note that $\hat{S}_y - \hat{S}_z = -\mathbb{i}(\hat{c}_3^\dagger\hat{c}_1 - \hat{c}_1^\dagger\hat{c}_3) + \mathbb{i}(\hat{c}_1^\dagger\hat{c}_2 - \hat{c}_2^\dagger\hat{c}_1)$ conserves total particle number $\hat{N} \equiv \hat{n}_1+\hat{n}_2+\hat{n}_3 = \hat{c}_1^\dagger\hat{c}_1 + \hat{c}_2^\dagger\hat{c}_2 + \hat{c}_3^\dagger\hat{c}_3$, $[\hat{S}_y - \hat{S}_z, \hat{N}] = 0$. So $\hat{S}_y - \hat{S}_z$ is block diagonalized in the Fock space into subspaces with fixed total particle number.

0-particle space: one basis state $|\text{vac}\rangle$,

$|\text{vac}\rangle$ is an eigenstate of $\hat{S}_y - \hat{S}_z$ with eigenvalue 0.

1-particle space: three basis states $\hat{c}_1^\dagger|\text{vac}\rangle$, $\hat{c}_2^\dagger|\text{vac}\rangle$, $\hat{c}_3^\dagger|\text{vac}\rangle$,

under these basis, $\hat{S}_y - \hat{S}_z$ is $\begin{pmatrix} 0 & \mathbb{i} & \mathbb{i} \\ -\mathbb{i} & 0 & 0 \\ -\mathbb{i} & 0 & 0 \end{pmatrix}$, it has eigenvalues $-\sqrt{2}$, 0, $\sqrt{2}$.

2-particle space: use the basis and results in (b),

$\hat{S}_y - \hat{S}_z$ is $\begin{pmatrix} 0 & 0 & -\mathbb{i} \\ 0 & 0 & \mathbb{i} \\ \mathbb{i} & -\mathbb{i} & 0 \end{pmatrix}$, it has eigenvalues $-\sqrt{2}$, 0, $\sqrt{2}$.

3-particle space: one basis state $\hat{c}_1^\dagger \hat{c}_2^\dagger \hat{c}_3^\dagger |\text{vac}\rangle$,

$\hat{c}_1^\dagger \hat{c}_2^\dagger \hat{c}_3^\dagger |\text{vac}\rangle$ is an eigenstate of $\hat{S}_y - \hat{S}_z$ with eigenvalue 0.

Method #2: $\hat{S}_y - \hat{S}_z = (\hat{c}_1^\dagger, \hat{c}_2^\dagger, \hat{c}_3^\dagger) \begin{pmatrix} 0 & \mathbb{i} & \mathbb{i} \\ -\mathbb{i} & 0 & 0 \\ -\mathbb{i} & 0 & 0 \end{pmatrix} \begin{pmatrix} \hat{c}_1 \\ \hat{c}_2 \\ \hat{c}_3 \end{pmatrix}$. The 3×3 hermitian matrix in the middle has eigenvalues $-\sqrt{2}, 0, +\sqrt{2}$. Then $\begin{pmatrix} 0 & \mathbb{i} & \mathbb{i} \\ -\mathbb{i} & 0 & 0 \\ -\mathbb{i} & 0 & 0 \end{pmatrix} = U \cdot \begin{pmatrix} -\sqrt{2} & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & \sqrt{2} \end{pmatrix} \cdot U^\dagger$. Here U is a 3×3 unitary matrix. Because we do not need the eigenstates, we do not need to solve U.

Define $(\hat{c}_1'^\dagger, \hat{c}_2'^\dagger, \hat{c}_3'^\dagger) = (\hat{c}_1^\dagger, \hat{c}_2^\dagger, \hat{c}_3^\dagger) \cdot U$, then $\{\hat{c}_i', \hat{c}_j'^\dagger\} = \delta_{i,j}$, and $\mathbb{i}\hat{S}_y + \mathbb{i}\hat{S}_z = -\sqrt{2} \cdot \hat{n}_1' + 0 \cdot \hat{n}_2' + \sqrt{2} \cdot \hat{n}_3'$, where $\hat{n}_i' \equiv \hat{c}_i'^\dagger \hat{c}_i'$ is the occupation number operator in the new basis. This basis change does not change the fermion vacuum.

Therefore the occupation basis $|n_1', n_2', n_3'\rangle = (\hat{c}_1'^\dagger)^{n_1'} (\hat{c}_2'^\dagger)^{n_2'} (\hat{c}_3'^\dagger)^{n_3'} |\text{vac}\rangle$ are normalized eigenstates of $\mathbb{i}\hat{S}_y + \mathbb{i}\hat{S}_z$, with eigenvalues $-\sqrt{2} \cdot n_1' + 0 \cdot n_2' + \sqrt{2} \cdot n_3'$, where $n_{1,2,3}' = 0$ or 1.

Method #2++: use the result of (c), $\exp(\mathbb{i}\frac{\pi}{4}\hat{S}_x) \cdot (\hat{S}_y - \hat{S}_z) \cdot \exp(-\mathbb{i}\frac{\pi}{4}\hat{S}_x) = -\sqrt{2}\hat{S}_z$.

Because $\exp(\mathbb{i}\frac{\pi}{4}\hat{S}_x)$ is a unitary operator, $-\sqrt{2}\hat{S}_z$ has the same eigenvalues as $\hat{S}_y - \hat{S}_z$.

$-\sqrt{2}\hat{S}_z = (\hat{c}_1^\dagger, \hat{c}_2^\dagger, \hat{c}_3^\dagger) \begin{pmatrix} 0 & \sqrt{2}\mathbb{i} & 0 \\ -\sqrt{2}\mathbb{i} & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \hat{c}_1 \\ \hat{c}_2 \\ \hat{c}_3 \end{pmatrix}$. It should be easier to obtain the eigenvalues of the 3×3 matrix in the middle (only need to diagonalize the top-left 2×2 block). Then this proceeds in the same way as the previous method.

(e) Method #1: brute-force diagonalization.

Note that $\hat{H}$ does NOT conserve total particle number under $\hat{c}$ basis, but can change total particle number by ± 2.

Arrange the 8 occupation basis $|n_1, n_2, n_3\rangle$ in the following order (the first four states have even particle number, the last four states have odd particle number),

$|0,0,0\rangle = |\text{vac}\rangle$, $|0,1,1\rangle$, $|1,0,1\rangle$, $|1,1,0\rangle$, $|1,1,1\rangle$, $|1,0,0\rangle$, $|0,1,0\rangle$, $|0,0,1\rangle$.

The Hamiltonian is block-diagonalized into two 4×4 blocks,

$$H = \begin{pmatrix} 0 & 1 & 1 & 0 & & & & \\ 1 & 1 & 1 & 0 & & & & \\ 1 & 1 & 1 & 0 & & & & \\ 0 & 0 & 0 & 0 & & & & \\ & & & & 1 & 1 & -1 & 0 \\ & & & & 1 & 0 & 1 & 0 \\ & & & & -1 & 1 & 0 & 0 \\ & & & & 0 & 0 & 0 & 1 \end{pmatrix}.$$ Be careful about the fermion exchange signs.

So $|1,1,0\rangle$ is an eigenstate with eigenvalue 0. $|0,0,1\rangle$ is an eigenstate with eigenvalue -1.

The 3×3 matrix $\begin{pmatrix} 0 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{pmatrix}$, with basis $(|0,0,0\rangle, |0,1,1\rangle, |1,0,1\rangle)$, has eigenvalues

$1+\sqrt{3}$ with un-normalized eigenvector $(\sqrt{3}-1, 1, 1)^T$;

$1-\sqrt{3}$ with un-normalized eigenvector $(-\sqrt{3}-1, 1, 1)^T$;

and 0 with un-normalized eigenvector $(0, 1, -1)^T$.

The 3×3 matrix $\begin{pmatrix} 1 & 1 & -1 \\ 1 & 0 & 1 \\ -1 & 1 & 0 \end{pmatrix}$, with basis $(|1,1,1\rangle, |1,0,0\rangle, |0,1,0\rangle)$, has eigenvalues

$-\sqrt{3}$ with un-normalized eigenvector $(\sqrt{3}-1, -1, 1)^T$;

$\sqrt{3}$ with un-normalized eigenvector $(-\sqrt{3}-1, -1, 1)^T$;

and 1 with un-normalized eigenvector $(0, 1, 1)^T$.

The normalized eigenstates are omitted here.

Method #2: use symmetry and particle-hole transformation.

$\hat{H}$ does not change if we exchange $\hat{c}_1 \leftrightarrow \hat{c}_2$ ($\hat{c}_1^\dagger \leftrightarrow \hat{c}_2^\dagger$).

Define $\hat{c'}_1 = \frac{1}{\sqrt{2}}(\hat{c}_1 - \hat{c}_2)$, $\hat{c'}_2 = \frac{1}{\sqrt{2}}(\hat{c}_1 + \hat{c}_2)$, $\hat{c'}_3 = \hat{c}_3^\dagger$. They satisfy the canonical anti-commutation relations, $\{\hat{c'}_i, \hat{c'}^\dagger_j\} = \delta_{i,j}$ and $\{\hat{c'}_i, \hat{c'}_j\} = 0$.

Because of the particle-hole transformation on the 3rd fermion mode, the new "vacuum" is $|\text{vac}'\rangle = \hat{c}_3^\dagger|\text{vac}\rangle$.

$\hat{H} = -\hat{c'}^\dagger_1\hat{c'}_1 + \hat{c'}^\dagger_2\hat{c'}_2 - \hat{c'}^\dagger_3\hat{c'}_3 + 1 + \sqrt{2}\cdot(\hat{c'}^\dagger_3\hat{c'}_2 + \hat{c'}^\dagger_2\hat{c'}_3)$.

Note that $\hat{H}$ conserves total 'particle number' $\hat{n}' = \hat{n'}_1 + \hat{n'}_2 + \hat{n'}_3$ under the $\hat{c}'$ basis. And it also conserves $\hat{n'}_1$.

In the $\hat{n'} = 0$ subspace, the basis $|\text{vac}'\rangle = \hat{c}_3^\dagger|\text{vac}\rangle$ is an eigenstate with eigenvalue 1.

In the $\hat{n'} = 3$ subspace, the basis $|n_1' = 1, n_2' = 1, n_3' = 1\rangle = \hat{c}_1^\dagger \hat{c}_2^\dagger|\text{vac}\rangle$ is an eigenstate with eigenvalue 0.

In the $\hat{n'} = 1$ subspace with basis

$|n_1' = 1, n_2' = 0, n_3' = 0\rangle$, $|n_1' = 0, n_2' = 1, n_3' = 0\rangle$, $|n_1' = 0, n_2' = 0, n_3' = 1\rangle$, the Hamiltonian is $\begin{pmatrix} 0 & 0 & 0 \\ 0 & 2 & \sqrt{2} \\ 0 & \sqrt{2} & 0 \end{pmatrix}$, with eigenvalues 0, $1+\sqrt{3}$, $1-\sqrt{3}$, and corresponding un-normalized eigenvectors $(1,0,0)^T$, $(0, 1+\sqrt{3}, \sqrt{2})^T$, $(0, 1-\sqrt{3}, \sqrt{2})^T$.

In the $\hat{n'} = 2$ subspace with basis

$|n_1' = 0, n_2' = 1, n_3' = 1\rangle$, $|n_1' = 1, n_2' = 0, n_3' = 1\rangle$, $|n_1' = 1, n_2' = 1, n_3' = 0\rangle$, the Hamiltonian is $\begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & \sqrt{2} \\ 0 & \sqrt{2} & 1 \end{pmatrix}$, with eigenvalues 1, $+\sqrt{3}$, $-\sqrt{3}$, and corresponding un-normalized eigenvectors $(1,0,0)^T$, $(0, \sqrt{2}, 1+\sqrt{3})^T$, $(0, \sqrt{2}, 1-\sqrt{3})^T$.

Method #2++: the Hamiltonian in method #2 can be further diagonalized.

$\hat{H} = -\hat{n'}_1 + 1 + \begin{pmatrix} \hat{c'}_2^\dagger & \hat{c'}_3^\dagger \end{pmatrix} \cdot \begin{pmatrix} 1 & \sqrt{2} \\ \sqrt{2} & -1 \end{pmatrix} \cdot \begin{pmatrix} \hat{c'}_2 \\ \hat{c'}_3 \end{pmatrix}$.

The 2×2 matrix $\begin{pmatrix} 1 & \sqrt{2} \\ \sqrt{2} & -1 \end{pmatrix}$ has eigenvalues $\pm\sqrt{3}$. It can be diagonalized by a 2×2 unitary matrix $U = \begin{pmatrix} \frac{1}{\sqrt{3-\sqrt{3}}} & -\frac{1}{\sqrt{3+\sqrt{3}}} \\ \frac{1}{\sqrt{3+\sqrt{3}}} & \frac{1}{\sqrt{3-\sqrt{3}}} \end{pmatrix}$, with $\begin{pmatrix} 1 & \sqrt{2} \\ \sqrt{2} & -1 \end{pmatrix} = U \cdot \begin{pmatrix} \sqrt{3} & 0 \\ 0 & -\sqrt{3} \end{pmatrix} \cdot U^\dagger$.

Define $\hat{c''}_1 = \hat{c'}_1$, $\begin{pmatrix} \hat{c''}_2 \\ \hat{c''}_3 \end{pmatrix} = U^\dagger \cdot \begin{pmatrix} \hat{c'}_2 \\ \hat{c'}_3 \end{pmatrix}$. This is a unitary transformation without particle-hole transformation. The "vacuum" of $\hat{c''}$ is the same as the "vacuum" of $\hat{c'}$, $|\text{vac}''\rangle = |\text{vac}'\rangle = \hat{c}_3^\dagger|\text{vac}\rangle$.

The Hamiltonian becomes a linear combination of occupation number operators,

$\hat{H} = -\hat{n''}_1 + 1 + \sqrt{3}\hat{n''}_2 - \sqrt{3}\hat{n''}_3$.

Then the $\hat{c''}$ occupation basis, $|n_1'', n_2'', n_3''\rangle = (\hat{c''}_1^\dagger)^{n_1''}(\hat{c''}_2^\dagger)^{n_2''}(\hat{c''}_3^\dagger)^{n_3''}|\text{vac}''\rangle$, are the eigenstates of $\hat{H}$, with eigenvalues $(-n_1'' + 1 + \sqrt{3}n_2'' - \sqrt{3}n_3'')$, where $n_{1,2,3}'' = 0$ or 1.

4. Second quantization: identical non-interacting particles in 1D harmonic potential. Subscript $_{\text{1-body}}$ ($_{\text{Fock}}$) indicates operators for single-particle (in Fock space).

The single-particle Hamiltonian is $\hat{H}_{\text{1-body}} = \frac{\hat{p}^2_{\text{1-body}}}{2m} + \frac{m\omega^2}{2}\hat{x}^2_{\text{1-body}}$ [action on single-particle wavefunctions is $\hat{H}_{\text{1-body}}\,\psi(x) = (-\frac{\hbar^2}{2m}\partial_x^2 + \frac{m\omega^2}{2}x^2)\,\psi(x)$], with normalized single-particle ground state $|\psi_0\rangle$ [wavefunction $\psi_0(x) \equiv \langle x|\psi_0\rangle = (\frac{m\omega}{\hbar\pi})^{1/4}\exp(-\frac{x^2}{2\hbar/m\omega})$], and normalized excited states $|\psi_n\rangle = \frac{1}{\sqrt{n!}}(\hat{a}^\dagger_{\text{1-body}})^n|\psi_0\rangle$. Here $\hat{a}^\dagger_{\text{1-body}} = \frac{m\omega\hat{x}-\mathrm{i}\hat{p}}{\sqrt{2m\omega\hbar}}$, $[\hat{a}_{\text{1-body}}, \hat{a}^\dagger_{\text{1-body}}] = 1$, and $\hat{H}_{\text{1-body}} = \hbar\omega\cdot(\hat{a}^\dagger_{\text{1-body}}\hat{a}_{\text{1-body}}+\frac{1}{2})$. The single-particle energy eigenvalues are $E_n = \hbar\omega\cdot(n+\frac{1}{2})$ for state $|\psi_n\rangle$, $n = 0, 1, \ldots$.

Denote the creation (annihilation) operators for single-particle states $|\psi_n\rangle$ by $\widehat{\psi_n}^\dagger$ ($\widehat{\psi_n}$). We will consider the case of fermions, then $\{\widehat{\psi_n}, \widehat{\psi_m}^\dagger\} = \delta_{n,m}$, $\{\widehat{\psi_n}, \widehat{\psi_m}\} = 0$.

The 'second quantized' Hamiltonian for identical particles is $\hat{H}_{\text{Fock}} = \sum_{n=0}^\infty E_n\,\widehat{\psi_n}^\dagger\widehat{\psi_n}$. This can be 'derived' from $\hat{H}_{\text{Fock}} = \int \mathrm{d}x\,\widehat{\psi(x)}^\dagger\cdot(-\frac{\hbar^2\partial_x^2}{2m} + \frac{m\omega^2x^2}{2})\cdot\widehat{\psi(x)}$. Here $\widehat{\psi(x)}^\dagger$ is the creation operator for position eigenbasis $|x\rangle$, and $\widehat{\psi(x)}^\dagger = \sum_{n=0}^\infty \widehat{\psi_n}^\dagger\langle\psi_n|x\rangle$. Then $\hat{H}_{\text{Fock}}$
$= \int \mathrm{d}x\,\sum_{n=0}^\infty \widehat{\psi_n}^\dagger\langle\psi_n|x\rangle\cdot(-\frac{\hbar^2\partial_x^2}{2m} + \frac{m\omega^2x^2}{2})\cdot\sum_{n'=0}^\infty\langle x|\psi_{n'}\rangle\widehat{\psi_{n'}}$
$= \sum_{n,n'=0}^\infty\int \mathrm{d}x\,\widehat{\psi_n}^\dagger\langle\psi_n|x\rangle\cdot E_{n'}\cdot\langle x|\psi_{n'}\rangle\widehat{\psi_{n'}} = \sum_{n,n'=0}^\infty\widehat{\psi_n}^\dagger\cdot E_{n'}\delta_{n,n'}\cdot\widehat{\psi_{n'}} = \sum_{n=0}^\infty E_n\widehat{\psi_n}^\dagger\widehat{\psi_n}$.

(a) (5pts) Consider the ground state for two fermions, $|\psi^{(N=2)}_{\text{GS}}\rangle$. *Write down this state (in terms of* $\widehat{\psi_n}^\dagger$ *and the fermion vacuum* $|vac\rangle$*) and its energy. Write down the explicit two particle wavefunction* $\psi^{(N=2)}_{GS}(x_1, x_2)$*, and compute the expectation value of* $(x_1 - x_2)^2$.

(b) (5pts) *Derive the 'second quantized' form of* $\hat{x}_{Fock} \equiv \int \mathrm{d}x\,\widehat{\psi(x)}^\dagger\cdot x\cdot\widehat{\psi(x)}$ *and* $\hat{p}_{Fock} \equiv \int \mathrm{d}x\,\widehat{\psi(x)}^\dagger\cdot(-\mathrm{i}\hbar\partial_x)\cdot\widehat{\psi(x)}$*, in terms of* $\widehat{\psi_n}^\dagger$ *and* $\widehat{\psi_n}$*. Compute the commutator* $[\hat{x}_{Fock}, \hat{p}_{Fock}]$. [Hint: represent x and $-\mathrm{i}\hbar\partial_x$ by ladder operators for 1-body wavefunctions]

(c) (5pts) *Derive the 'second quantized' form of the two-body term* $\hat{V}(x_1, x_2) = (x_1-x_2)^2$, $\hat{V}_{Fock} = \frac{1}{2}\int \mathrm{d}x\int \mathrm{d}x'\,\widehat{\psi(x)}^\dagger\widehat{\psi(x')}^\dagger\cdot(x-x')^2\cdot\widehat{\psi(x')}\widehat{\psi(x)}$*, in terms of* $\widehat{\psi_n}^\dagger$ *and* $\widehat{\psi_n}$*. Check that this produces the same expectation value on the state in (a) as the result of (a).* [Hint: use ladder operators for x and x'.]

Solution:

(a) The two-fermion ground state is $|\psi^{(N=2)}_{\text{GS}}\rangle = \widehat{\psi_0}^\dagger\widehat{\psi_1}^\dagger|\text{vac}\rangle$.

Its energy is $E^{(N=2)}_{\text{GS}} = E_0\cdot 1 + E_1\cdot 1 = \hbar\omega\cdot 2$. [$\hat{H}_{\text{Fock}}|\psi^{(N=2)}_{\text{GS}}\rangle = E^{(N=2)}_{\text{GS}}|\psi^{(N=2)}_{\text{GS}}\rangle$.]

Its wavefunction is $\psi_{\text{GS}}^{(N=2)}(x_1, x_2) = \frac{1}{\sqrt{2}}[\psi_0(x_1)\psi_1(x_2) - \psi_0(x_2)\psi_1(x_1)]$, use $\psi_1(x) = (\frac{m\omega}{\hbar\pi})^{1/4}\frac{\sqrt{2}x}{\sqrt{\hbar/m\omega}}\exp(-\frac{x^2}{2\hbar/m\omega})$, we have $\psi_{\text{GS}}^{(N=2)}(x_1, x_2) = \sqrt{\frac{m\omega}{\hbar\pi}}(\frac{x_2-x_1}{\sqrt{\hbar/m\omega}})\exp(-\frac{x_1^2+x_2^2}{2\hbar/m\omega})$.

The expectation value of $(x_1 - x_2)^2$ is, $\int dx_1 \int dx_2\, (x_1 - x_2)^2 \cdot \frac{m\omega}{\hbar\pi}\frac{(x_2-x_1)^2}{\hbar/m\omega}\exp(-\frac{x_1^2+x_2^2}{\hbar/m\omega})$ $= \frac{m\omega}{\hbar} \cdot [2\langle x^4\rangle_{\psi_0} + 6(\langle x^2\rangle_{\psi_0})^2] = \frac{m\omega}{\hbar} \cdot 12(\langle x^2\rangle_{\psi_0})^2 = 3\frac{\hbar}{m\omega}$. Here $\langle\cdot\rangle_{\psi_0}$ is the expectation value in the single-particle ground state ψ_0, $\langle x^2\rangle_{\psi_0} = \frac{\hbar}{2m\omega}$, and the Wick expansion result $\langle x^4\rangle_{\psi_0} = 3\langle x^2\rangle_{\psi_0}\langle x^2\rangle_{\psi_0}$ has been used.

(b) (steps omitted)

$\hat{x}_{\text{Fock}} = \sqrt{\frac{\hbar}{2m\omega}} \cdot \sum_{n=0}^{\infty}(\sqrt{n+1}\widehat{\psi_n}^\dagger\widehat{\psi_{n+1}} + \sqrt{n+1}\widehat{\psi_{n+1}}^\dagger\widehat{\psi_n})$.

$\hat{p}_{\text{Fock}} = -\mathbb{i}\sqrt{\frac{\hbar m\omega}{2}} \cdot \sum_{n=0}^{\infty}(\sqrt{n+1}\widehat{\psi_n}^\dagger\widehat{\psi_{n+1}} - \sqrt{n+1}\widehat{\psi_{n+1}}^\dagger\widehat{\psi_n})$.

These can be derived in similar way as $\hat{H}_{\text{Fock}}$, using

$\hat{x}_{\text{1-body}}\psi_n = \sqrt{\frac{\hbar}{2m\omega}}(\hat{a}_{\text{1-body}} + \hat{a}_{\text{1-body}}^\dagger)\psi_n = \sqrt{\frac{\hbar}{2m\omega}}(\sqrt{n}\psi_{n-1} + \sqrt{n+1}\psi_{n+1})$, and

$\hat{p}_{\text{1-body}}\psi_n = -\mathbb{i}\sqrt{\frac{\hbar m\omega}{2}}(\hat{a}_{\text{1-body}} - \hat{a}_{\text{1-body}}^\dagger)\psi_n = -\mathbb{i}\sqrt{\frac{\hbar m\omega}{2}}(\sqrt{n}\psi_{n-1} - \sqrt{n+1}\psi_{n+1})$.

Note that these result can be obtained by the following empirical rule: represent the single-particle operator $\hat{O}_{\text{1-body}}$ by $\sum_{n,n'}|\psi_n\rangle O_{n,n'}\langle\psi_n'|$, where $O_{n,n'} = \langle\psi_n|\hat{O}_{\text{1-body}}|\psi_{n'}\rangle$, then 'promote' $|\psi_n\rangle$ to $\widehat{\psi_n}^\dagger$, and $\langle\psi_{n'}|$ to $\widehat{\psi_{n'}}$. The operator in Fock space is then $\hat{O}_{\text{Fock}} = \sum_{n,n'}\widehat{\psi_n}^\dagger O_{n,n'}\widehat{\psi_{n'}}$.

Use $[\hat{A}\hat{B}, \hat{C}\hat{D}] = \hat{A}\{\hat{B}, \hat{C}\}\hat{D} - \{\hat{A}, \hat{C}\}\hat{B}\hat{D} + \hat{C}\hat{A}\{\hat{B}, \hat{D}\} - \hat{C}\{\hat{A}, \hat{D}\}\hat{B}$.

$[\hat{x}_{\text{Fock}}, \hat{p}_{\text{Fock}}] = -\mathbb{i}\frac{\hbar}{2}\sum_{n,n'=0}^{\infty}\sqrt{(n+1)(n'+1)}\Big($
$(\delta_{n+1,n'}\widehat{\psi_n}^\dagger\widehat{\psi_{n'+1}} - 0 + 0 - \delta_{n,n'+1}\widehat{\psi_{n'}}^\dagger\widehat{\psi_{n+1}})$
$-(\delta_{n+1,n'+1}\widehat{\psi_n}^\dagger\widehat{\psi_{n'}} - 0 + 0 - \delta_{n,n'}\widehat{\psi_{n'+1}}^\dagger\widehat{\psi_{n+1}})$
$+(\delta_{n,n'}\widehat{\psi_{n+1}}^\dagger\widehat{\psi_{n'+1}} - 0 + 0 - \delta_{n+1,n'+1}\widehat{\psi_{n'}}^\dagger\widehat{\psi_n})$
$-(\delta_{n,n'+1}\widehat{\psi_{n+1}}^\dagger\widehat{\psi_{n'}} - 0 + 0 - \delta_{n+1,n'}\widehat{\psi_{n'+1}}^\dagger\widehat{\psi_n})\Big)$
$= \mathbb{i}\hbar \cdot \sum_{n=0}^{\infty}\widehat{\psi_n}^\dagger\widehat{\psi_n}$.

Note that $\sum_{n=0}^{\infty}\widehat{\psi_n}^\dagger\widehat{\psi_n}$ is the total particle number operator in Fock space.

(c) (steps omitted)

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

$+\left(\sqrt{(m+2)(m+1)}\left(\widehat{\psi_n}^\dagger\widehat{\psi_m}^\dagger\widehat{\psi_{m+2}}\widehat{\psi_n}+\widehat{\psi_n}^\dagger\widehat{\psi_{m+2}}^\dagger\widehat{\psi_m}\widehat{\psi_n}\right)+(2m+1)\widehat{\psi_n}^\dagger\widehat{\psi_m}^\dagger\widehat{\psi_m}\widehat{\psi_n}\right)\Big]$

[note: the three $(\dots)$ terms inside the summation are from x^2, $-2xx'$, x'^2, in $\frac{1}{2}\int \mathrm{d}x \int \mathrm{d}x' \, \widehat{\psi(x)}^\dagger \widehat{\psi(x')}^\dagger \cdot (x-x')^2 \cdot \widehat{\psi(x')}\widehat{\psi(x)}$, respectively]

Acting $\hat{V}_{\text{Fock}}$ on $|\psi_{\text{GS}}^{(N=2)}\rangle = \widehat{\psi_0}^\dagger\widehat{\psi_1}^\dagger|\text{vac}\rangle$, the coefficient of $\widehat{\psi_0}^\dagger\widehat{\psi_1}^\dagger|\text{vac}\rangle$ in the result is the expectation value, and it is $\frac{\hbar}{4m\omega}(0+0+(1+3)-0-2\cdot(-1)-2\cdot(-1)-0+0+0+(3+1)) = \frac{3\hbar}{m\omega}$. Here $(1+3)$ is from the $(2n+1)\widehat{\psi_n}^\dagger\widehat{\psi_m}^\dagger\widehat{\psi_m}\widehat{\psi_n}$ term with $(n,m)=(0,1)$ and $(n,m)=(1,0)$; (-1) is from the $\widehat{\psi_n}^\dagger\widehat{\psi_{m+1}}^\dagger\widehat{\psi_m}\widehat{\psi_{n+1}}$ and $\widehat{\psi_{n+1}}^\dagger\widehat{\psi_m}^\dagger\widehat{\psi_{m+1}}\widehat{\psi_n}$ terms with $(n,m)=(0,0)$.

empirical rule for two-particle operator:

if $\hat{O}_{\text{2-body}} = \sum_{n,m,n',m'} |\psi_n \otimes \psi_m\rangle O_{n,m,n',m'} \langle \psi_{n'} \otimes \psi_{m'}|$, where $|\psi_{n'} \otimes \psi_{m'}\rangle$ is the tensor product basis state, then the 'second quantized' form is $\hat{O}_{\text{Fock}} = \frac{1}{2}\sum_{n,m,n',m'} \widehat{\psi_n}^\dagger\widehat{\psi_m}^\dagger O_{n,m,n',m'}\widehat{\psi_{m'}}\widehat{\psi_{n'}}$. NOTE the 'normal ordering' of creation/annihilation operators.