

Homework #2: Brief solutions

***** (about lecture #1) *****

1. (5pts) The definition of unitary operator is that a linear operator \hat{U} is unitary if the inner product $(\hat{U}\phi, \hat{U}\psi) = (\phi, \psi)$ for any states ϕ and ψ . *Prove that this condition is equivalent to: $(\hat{U}\psi, \hat{U}\psi) = (\psi, \psi)$ for any state ψ .* [Hint: the former condition obviously imply the latter one, try to derive the former condition from the latter one, by assuming an arbitrary linear combination of states]

Solutions:

Consider the inner product $(c_1\phi + c_2\psi, c_1\phi + c_2\psi) = (c_1^*, c_2^*) \begin{pmatrix} \langle\phi|\phi\rangle, & \langle\phi|\psi\rangle \\ \langle\psi|\phi\rangle, & \langle\psi|\psi\rangle \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \end{pmatrix}$, where $c_{1,2}$ are two complex numbers, ϕ, ψ are two quantum states.

$$\text{According to the latter condition, this equals to } (\hat{U}(c_1\phi + c_2\psi), \hat{U}(c_1\phi + c_2\psi)) \\ = (c_1^*, c_2^*) \begin{pmatrix} \langle\hat{U}\phi|\hat{U}\phi\rangle, & \langle\hat{U}\phi|\hat{U}\psi\rangle \\ \langle\hat{U}\psi|\hat{U}\phi\rangle, & \langle\hat{U}\psi|\hat{U}\psi\rangle \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = (c_1^*, c_2^*) \begin{pmatrix} \langle\phi|\phi\rangle, & \langle\hat{U}\phi|\hat{U}\psi\rangle \\ \langle\hat{U}\psi|\hat{U}\phi\rangle, & \langle\psi|\psi\rangle \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \end{pmatrix}.$$

Then we have, $c_1^*c_2\langle\phi|\psi\rangle + c_2^*c_1\langle\psi|\phi\rangle = c_1^*c_2\langle\hat{U}\phi|\hat{U}\psi\rangle + c_2^*c_1\langle\hat{U}\psi|\hat{U}\phi\rangle$.

Choose $c_1 = c_2 = 1$, this condition is, $2 \cdot \text{Re}(\langle\phi|\psi\rangle) = 2 \cdot \text{Re}(\langle\hat{U}\phi|\hat{U}\psi\rangle)$;

choose $c_1 = i, c_2 = 1$, this is, $2 \cdot \text{Im}(\langle\phi|\psi\rangle) = 2 \cdot \text{Im}(\langle\hat{U}\phi|\hat{U}\psi\rangle)$.

Here Re and Im denote the real and imaginary parts of a complex number, respectively.

Therefore $\langle\phi|\psi\rangle = \langle\hat{U}\phi|\hat{U}\psi\rangle$.

2. \mathcal{H}_1 and \mathcal{H}_2 are both 2-dimensional Hilbert spaces. \mathcal{H}_1 has complete orthonormal basis $|e_1\rangle$ and $|e_2\rangle$, \mathcal{H}_2 has complete orthonormal basis $|e'_1\rangle$ and $|e'_2\rangle$. In the following we will represent operators in \mathcal{H}_1 and \mathcal{H}_2 as matrices under these basis. Define three nontrivial hermitian operators $\hat{\sigma}_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$, $\hat{\sigma}_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$, $\hat{\sigma}_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$, in \mathcal{H}_1 ; and $\hat{\sigma}'_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$, $\hat{\sigma}'_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$, $\hat{\sigma}'_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$, in \mathcal{H}_2 .

(a) (5pts) Consider a state in the 4-dimensional Hilbert space $\mathcal{H}_1 \otimes \mathcal{H}_2$ described by the density matrix $\hat{\rho} = \frac{1}{4}\mathbb{1}_{4 \times 4} + \frac{1}{8}\hat{\sigma}_3 \otimes \hat{\sigma}'_3 + \frac{1}{8}\hat{\sigma}_1 \otimes \hat{\sigma}'_1$, where $\mathbb{1}_{4 \times 4}$ is the 4×4 identity matrix(identity operator in $\mathcal{H}_1 \otimes \mathcal{H}_2$). *Compute the eigenvalues and orthonormal eigenstates*

of ρ . [Hint: facts about Pauli matrices in Homework#1 might help]

(b) (5pts) Check that $\hat{\rho}$ defined in (a) is a legitimate density matrix, namely that it is hermitian, positive semi-definite, and has unity trace. Check that whether $\hat{\rho}$ represents a pure state or not. Compute the von Neumann entropy $S[\hat{\rho}] \equiv -\text{Tr}[\hat{\rho} \log \hat{\rho}]$. [Hint: result of (a) is of course useful]

(c) (5pts) Consider an observable $\hat{O} = \hat{\sigma}_2 \otimes \hat{\sigma}'_2$ defined on $\mathcal{H}_1 \otimes \mathcal{H}_2$. Measure \hat{O} under the state $\hat{\rho}$ defined in (a). What are the possible measurement results, and their corresponding probabilities? For each possible measurement result, what is the density matrix for the collapsed state after measurement? [Hint: check that $[\hat{\rho}, \hat{O}] = 0$, this fact might help]

(d) (5pts) Consider an observable $\hat{Q} = \hat{\sigma}_2 \otimes \mathbb{1}_{2 \times 2}$ defined on $\mathcal{H}_1 \otimes \mathcal{H}_2$. Here $\mathbb{1}_{2 \times 2}$ is the 2×2 identity matrix. Measure \hat{Q} under the state $\hat{\rho}$ defined in (a). What are the possible measurement results, and their corresponding probabilities? For each possible measurement result, what is the density matrix for the collapsed state after measurement?

Solutions:

(a) Under the basis $(|e_1 \otimes e'_1\rangle, |e_1 \otimes e'_2\rangle, |e_2 \otimes e'_1\rangle, |e_2 \otimes e'_2\rangle)$, $\hat{\rho}$ is
$$\begin{pmatrix} \frac{3}{8} & 0 & 0 & \frac{1}{8} \\ 0 & \frac{1}{8} & \frac{1}{8} & 0 \\ 0 & \frac{1}{8} & \frac{1}{8} & 0 \\ \frac{1}{8} & 0 & 0 & \frac{3}{8} \end{pmatrix}.$$

This is block-diagonalized, similar to Homework #1 Problem 7(a). Rearrange the basis into $(|e_1 \otimes e'_1\rangle, |e_2 \otimes e'_2\rangle, |e_1 \otimes e'_2\rangle, |e_2 \otimes e'_1\rangle)$, this matrix becomes
$$\begin{pmatrix} \frac{3}{8} & \frac{1}{8} & 0 & 0 \\ \frac{1}{8} & \frac{3}{8} & 0 & 0 \\ 0 & 0 & \frac{1}{8} & \frac{1}{8} \\ 0 & 0 & \frac{1}{8} & \frac{1}{8} \end{pmatrix}.$$

The top-left 2×2 block has eigenvalue $\frac{3}{8} + \frac{1}{8} = \frac{1}{2}$ for eigenvector $\frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}$, and eigenvalue $\frac{3}{8} - \frac{1}{8} = \frac{1}{4}$ for eigenvector $\frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix}$.

The bottom-right 2×2 block has eigenvalue $\frac{1}{8} + \frac{1}{8} = \frac{1}{4}$ for eigenvector $\frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}$, and eigenvalue $\frac{1}{8} - \frac{1}{8} = 0$ for eigenvector $\frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix}$.

The final results are

eigenvalue of $\hat{\rho}$	eigenstate of $\hat{\rho}$
$\frac{1}{2}$	$\frac{1}{\sqrt{2}}(e_1 \otimes e'_1\rangle + e_2 \otimes e'_2\rangle)$
$\frac{1}{4}$	$\frac{1}{\sqrt{2}}(e_1 \otimes e'_1\rangle - e_2 \otimes e'_2\rangle)$
$\frac{1}{4}$	$\frac{1}{\sqrt{2}}(e_1 \otimes e'_2\rangle + e_2 \otimes e'_1\rangle)$
0	$\frac{1}{\sqrt{2}}(e_1 \otimes e'_2\rangle - e_2 \otimes e'_1\rangle)$

Method #2 for eigenvalues: not rigorous.

The three terms in $\hat{\rho}$ mutually commute, in particular $(\hat{\sigma}_3 \otimes \hat{\sigma}_3) \cdot (\hat{\sigma}_1 \otimes \hat{\sigma}_1) = -\hat{\sigma}_2 \otimes \hat{\sigma}_2 = (\hat{\sigma}_1 \otimes \hat{\sigma}_1) \cdot (\hat{\sigma}_3 \otimes \hat{\sigma}_3)$. So they can have simultaneous eigenstates.

$(\hat{\sigma}_3 \otimes \hat{\sigma}_3)$ has eigenvalues ± 1 , and $(\hat{\sigma}_1 \otimes \hat{\sigma}_1)$ has eigenvalue ± 1 . The 4 possible combinations of eigenvalues are $\frac{1}{4} + \frac{1}{8} + \frac{1}{8} = \frac{1}{2}$, $\frac{1}{4} + \frac{1}{8} - \frac{1}{8} = \frac{1}{4}$, $\frac{1}{4} - \frac{1}{8} + \frac{1}{8} = \frac{1}{4}$, $\frac{1}{4} - \frac{1}{8} - \frac{1}{8} = 0$.

But you still have to prove that each of these 4 combinations appear once.

(b) $\hat{\rho}$ is obviously hermitian, has non-negative eigenvalues (positive semi-definite), and unity trace (sum of eigenvalues equal unity).

$$S[\hat{\rho}] = -\sum \lambda \log(\lambda) = -\frac{1}{2} \log(\frac{1}{2}) - \frac{1}{4} \log(\frac{1}{4}) - \frac{1}{4} \log(\frac{1}{4}) - 0 \log(0) = \frac{3}{2} \log(2).$$

$\hat{\rho}$ is not a pure state (non-zero entropy, more-than-one nonzero eigenvalues).

(c) Under the basis $(|e_1 \otimes e'_1\rangle, |e_1 \otimes e'_2\rangle, |e_2 \otimes e'_1\rangle, |e_2 \otimes e'_2\rangle)$, \hat{O} is $\begin{pmatrix} 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{pmatrix}$. It is

easy to check that $[\hat{\rho}, \hat{O}] = 0$. In fact the eigenstates in (a) are also eigenstates of \hat{O} ,

eigenvalue of $\hat{\rho}$ (probability)	eigenstate of $\hat{\rho}$	eigenvalue of \hat{O}
$\frac{1}{2}$	$ \psi_1\rangle \equiv \frac{1}{\sqrt{2}}(e_1 \otimes e'_1\rangle + e_2 \otimes e'_2\rangle)$	-1
$\frac{1}{4}$	$ \psi_2\rangle \equiv \frac{1}{\sqrt{2}}(e_1 \otimes e'_1\rangle - e_2 \otimes e'_2\rangle)$	+1
$\frac{1}{4}$	$ \psi_3\rangle \equiv \frac{1}{\sqrt{2}}(e_1 \otimes e'_2\rangle + e_2 \otimes e'_1\rangle)$	+1
0	$ \psi_4\rangle \equiv \frac{1}{\sqrt{2}}(e_1 \otimes e'_2\rangle - e_2 \otimes e'_1\rangle)$	-1

Therefore the measurement result can be

-1 with probability $\frac{1}{2} + 0 = \frac{1}{2}$; and

$+1$ with probability $\frac{1}{4} + \frac{1}{4} = \frac{1}{2}$.

If the result is -1 , the collapsed state density matrix is $\frac{1}{\frac{1}{2}+0}(\frac{1}{2}|\psi_1\rangle\langle\psi_1| + 0|\psi_4\rangle\langle\psi_4|)$,

$$\begin{pmatrix} \frac{1}{2} & 0 & 0 & \frac{1}{2} \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ \frac{1}{2} & 0 & 0 & \frac{1}{2} \end{pmatrix} \text{ under the above basis, which becomes a pure state after measurement!}$$

If the result is $+1$, the collapsed state density matrix is $\frac{1}{\frac{1}{4}+\frac{1}{4}}(\frac{1}{4}|\psi_2\rangle\langle\psi_2| + \frac{1}{4}|\psi_3\rangle\langle\psi_3|)$,

$$\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 \\ 0 & 0 & \frac{1}{2} & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \text{ under the above basis, which is still a mixed state.}$$

(d) Under the basis $(|e_1 \otimes e'_1\rangle, |e_1 \otimes e'_2\rangle, |e_2 \otimes e'_1\rangle, |e_2 \otimes e'_2\rangle)$, \hat{Q} is
$$\begin{pmatrix} 0 & 0 & -i & 0 \\ 0 & 0 & 0 & -i \\ i & 0 & 0 & 0 \\ 0 & i & 0 & 0 \end{pmatrix}.$$

It has eigenvalues ± 1 (each is 2-fold degenerate). For eigenvalue $+1$, the two eigenstates can be chosen as $\frac{1}{\sqrt{2}}(|e_1\rangle + i|e_2\rangle) \otimes |e'_{1,2}\rangle$. For eigenvalue -1 , the two eigenstates can be chose as $\frac{1}{\sqrt{2}}(|e_1\rangle - i|e_2\rangle) \otimes |e'_{1,2}\rangle$.

The projection operator onto the eigenvalue $+1$ subspace is

$$\hat{P}_{\hat{Q}=+1} = \frac{1}{2}(|e_1\rangle + i|e_2\rangle)(\langle e_1| - i\langle e_2|) \otimes \mathbb{1}_{2 \times 2}, \text{ or } \frac{1}{2} \begin{pmatrix} 1 & 0 & -i & 0 \\ 0 & 1 & 0 & -i \\ i & 0 & 1 & 0 \\ 0 & i & 0 & 1 \end{pmatrix} \text{ under the above basis.}$$

The projection operator onto the eigenvalue -1 subspace is

$$\hat{P}_{\hat{Q}=-1} = \frac{1}{2}(|e_1\rangle - i|e_2\rangle)(\langle e_1| + i\langle e_2|) \otimes \mathbb{1}_{2 \times 2}, \text{ or } \frac{1}{2} \begin{pmatrix} 1 & 0 & i & 0 \\ 0 & 1 & 0 & i \\ -i & 0 & 1 & 0 \\ 0 & -i & 0 & 1 \end{pmatrix} \text{ under the above basis.}$$

The probability for getting measurement result $+1$ is $\text{Tr}(\hat{\rho}\hat{P}_{\hat{Q}=+1}) = \frac{1}{2}$, the collapsed state

is $\hat{P}_{\hat{Q}=+1}\hat{\rho}\hat{P}_{\hat{Q}=+1}/\text{Tr}(\hat{\rho}\hat{P}_{\hat{Q}=+1}) = \frac{1}{4} \begin{pmatrix} 1 & 0 & -i & 0 \\ 0 & 1 & 0 & -i \\ i & 0 & 1 & 0 \\ 0 & i & 0 & 1 \end{pmatrix}$, which is a mixed state.

The probability for getting measurement result -1 is $\text{Tr}(\hat{\rho}\hat{P}_{\hat{Q}=-1}) = \frac{1}{2}$, the collapsed state is $\hat{P}_{\hat{Q}=-1}\hat{\rho}\hat{P}_{\hat{Q}=-1}/\text{Tr}(\hat{\rho}\hat{P}_{\hat{Q}=-1}) = \frac{1}{4} \begin{pmatrix} 1 & 0 & i & 0 \\ 0 & 1 & 0 & i \\ -i & 0 & 1 & 0 \\ 0 & -i & 0 & 1 \end{pmatrix}$, which is a mixed state.

Method #2: brief descriptions only.

Once we know that \hat{Q} has only eigenvalues ± 1 , we can directly write down the projection operators, $\hat{P}_{\hat{Q}=+1} = \frac{1_{4 \times 4} + \hat{Q}}{2}$, $\hat{P}_{\hat{Q}=-1} = \frac{1_{4 \times 4} - \hat{Q}}{2}$.

We can then use $(\hat{A} \otimes \hat{B}) \cdot (\hat{C} \otimes \hat{D}) = (\hat{A}\hat{C}) \otimes (\hat{B}\hat{D})$, and $\text{Tr}_{\mathcal{H}_1 \otimes \mathcal{H}_2}(\hat{A} \otimes \hat{B}) = \text{Tr}_{\mathcal{H}_1}(\hat{A}) \cdot \text{Tr}_{\mathcal{H}_2}(\hat{B})$, and the multiplication rules of Pauli matrices, to do the remaining calculations.

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

3. Consider a single-boson Hilbert space with two complete orthonormal basis states, $|1\rangle$ & $|2\rangle$. Denote the corresponding creation, annihilation operators by $\hat{b}_1^\dagger, \hat{b}_1$ (for $|1\rangle$) and $\hat{b}_2^\dagger, \hat{b}_2$ (for $|2\rangle$), then $|1\rangle = \hat{b}_1^\dagger|\text{vac}\rangle$, $|2\rangle = \hat{b}_2^\dagger|\text{vac}\rangle$, where $|\text{vac}\rangle$ is the normalized ‘vacuum’ state, and $[\hat{b}_i, \hat{b}_j^\dagger] = \delta_{i,j}$, $[\hat{b}_i, \hat{b}_j] = [\hat{b}_i^\dagger, \hat{b}_j^\dagger] = 0$.

(a). (3pts) Write down a complete orthonormal basis for the Hilbert space of two bosons, in terms of tensor product states $|i\rangle \otimes |j\rangle$, $i, j = 1, 2$.

(b). (2pts) A unitary transformation \hat{U} is defined by its action on single-boson basis as: $|1\rangle \mapsto \hat{U}|1\rangle = (u|1\rangle - v|2\rangle)$, $|2\rangle \mapsto \hat{U}|2\rangle = (v^*|1\rangle + u^*|2\rangle)$, where u, v are two complex numbers and $|u|^2 + |v|^2 = 1$. Show that the above definition of \hat{U} is indeed a unitary transformation in single-boson Hilbert space.

(c). (5pts) The action of \hat{U} on a tensor product state will be transforming each of the

factors, for example $|1\rangle \otimes |2\rangle \mapsto \hat{U}|1\rangle \otimes \hat{U}|2\rangle$. Write down the transformation results of all two-boson basis in (a) induced by \hat{U} , as linear combinations of the original two-boson basis states. Explicitly show that this transformation in the two-boson Hilbert space is unitary.

(d). (5pts) \hat{U} can be extended to the entire Fock space as follows: The transformation of an operator \hat{O} by \hat{U} is formally $\hat{U}\hat{O}\hat{U}^\dagger$. We demand that the transformation results of \hat{b}_i^\dagger are: $\hat{U}\hat{b}_1^\dagger\hat{U}^\dagger = (u\hat{b}_1^\dagger - v\hat{b}_2^\dagger)$, and $\hat{U}\hat{b}_2^\dagger\hat{U}^\dagger = (v^*\hat{b}_1^\dagger + u^*\hat{b}_2^\dagger)$. Together with $\hat{U}|\text{vac}\rangle = |\text{vac}\rangle$, this can reproduce the definition of \hat{U} in single-boson space, e.g. $\hat{U}|1\rangle = \hat{U}\hat{b}_1^\dagger|\text{vac}\rangle = \hat{U}\hat{b}_1^\dagger\hat{U}^\dagger \cdot \hat{U}|\text{vac}\rangle = (u\hat{b}_1^\dagger - v\hat{b}_2^\dagger)|\text{vac}\rangle = u|1\rangle - v|2\rangle$. Use the creation operators to represent the two-boson basis in (a), then apply \hat{U} on them, represent the results as linear combinations of the original two-boson basis. The results should be consistent with (c).

(e). (5pts) Consider $\hat{H} = t \cdot (\hat{b}_1^\dagger\hat{b}_2 + \hat{b}_2^\dagger\hat{b}_1)$, where t is a real number. You can do a unitary transformation(basis change) to “diagonalize” \hat{H} : find a new set of orthonormal creation(annihilation) operators \hat{b}'_i (\hat{b}'_i) as linear combinations of \hat{b}_j^\dagger (\hat{b}_j), so that $\hat{H} = \epsilon_1\hat{b}'_1^\dagger\hat{b}'_1 + \epsilon_2\hat{b}'_2^\dagger\hat{b}'_2$, where $\epsilon_{1,2}$ are two c -numbers. These new operators should satisfy the same kind of commutation relations as the old ones, e.g. $[\hat{b}'_i, \hat{b}'_j^\dagger] = \delta_{i,j}$. Solve the new creation operators \hat{b}'_i^\dagger in terms of \hat{b}_j^\dagger , and solve $\epsilon_{1,2}$. Then write down all the eigenvalues and eigenstates of \hat{H} in the entire Fock space.

(f). (5pts) (DIFFICULT) The explicit form of operator \hat{U} in (d) in the entire Fock space is, $\hat{U} = \exp \left[i \sum_{i,j=1}^2 \hat{b}_i^\dagger (a_1\sigma_1 + a_2\sigma_2 + a_3\sigma_3)_{i,j} \hat{b}_j \right]$. Here $a_{1,2,3}$ are three real numbers, $\sigma_{1,2,3}$ are Pauli matrices defined in Homework #1 Problem 6. $(a_1\sigma_1 + a_2\sigma_2 + a_3\sigma_3)_{i,j}$ is the i^{th} -row- j^{th} -column element of the 2×2 matrix in the bracket. Solve the real numbers $a_{1,2,3}$ in terms of the complex numbers u, v used to define \hat{U} in (b). [Hint: compute $\hat{U}\hat{b}_{1,2}^\dagger\hat{U}^\dagger$ by the Baker-Hausdorff formula, compare the results with those in (d), some results in Homework #1 will be useful]

Solutions:

(a) by definition, the orthonormal occupation basis are,

$$\begin{aligned} |n_1 = 2, n_2 = 0\rangle &\equiv \frac{1}{\sqrt{2}}|1, 1\rangle \equiv \frac{1}{\sqrt{2}} \cdot \frac{1}{\sqrt{2}}(|1\rangle \otimes |1\rangle + |1\rangle \otimes |1\rangle) = |1\rangle \otimes |1\rangle, \\ |n_1 = 1, n_2 = 1\rangle &\equiv |1, 2\rangle \equiv \frac{1}{\sqrt{2}}(|1\rangle \otimes |2\rangle + |2\rangle \otimes |1\rangle), \\ |n_1 = 0, n_2 = 2\rangle &\equiv \frac{1}{\sqrt{2}}|2, 2\rangle \equiv \frac{1}{\sqrt{2}} \cdot \frac{1}{\sqrt{2}}(|2\rangle \otimes |2\rangle + |2\rangle \otimes |2\rangle) = |2\rangle \otimes |2\rangle. \end{aligned}$$

(b) one can check that $(\hat{U}|i\rangle, \hat{U}|j\rangle) = (|i\rangle, |j\rangle) = \delta_{i,j}$, for $i, j = 1, 2$.

$$(\hat{U}|1\rangle, \hat{U}|1\rangle) = (u|1\rangle - v|2\rangle, u|1\rangle - v|2\rangle) = u^*u + (-v)^*(-v) = 1,$$

$$(\hat{U}|1\rangle, \hat{U}|2\rangle) = (u|1\rangle - v|2\rangle, v^*|1\rangle + u^*|2\rangle) = u^*v^* + (-v)^*u^* = 0,$$

$$(\hat{U}|2\rangle, \hat{U}|1\rangle) = (\hat{U}|1\rangle, \hat{U}|2\rangle)^* = 0,$$

$$(\hat{U}|2\rangle, \hat{U}|2\rangle) = (v^*|1\rangle + u^*|2\rangle, v^*|1\rangle + u^*|2\rangle) = (v^*)^*(v^*) + (u^*)^*u^* = 1.$$

The action of \hat{U} on the 1-particle basis is, $(|1\rangle, |2\rangle) \mapsto (|1\rangle, |2\rangle) \begin{pmatrix} u & v^* \\ -v & u^* \end{pmatrix}$, it is also easy to check that the 2×2 matrix is unitary, under the condition that $|u|^2 + |v|^2 = 1$,

$$\begin{pmatrix} u & v^* \\ -v & u^* \end{pmatrix}^\dagger \cdot \begin{pmatrix} u & -v^* \\ v & u^* \end{pmatrix} = \begin{pmatrix} |u|^2 + |v|^2 & 0 \\ 0 & |u|^2 + |v|^2 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}.$$

(c) consider the basis in (a),

$$\begin{aligned} |1\rangle \otimes |1\rangle &\mapsto (u|1\rangle - v|2\rangle) \otimes (u|1\rangle - v|2\rangle) \\ &= u^2 \cdot |1\rangle \otimes |1\rangle - \sqrt{2}uv \cdot \frac{1}{\sqrt{2}}(|1\rangle \otimes |2\rangle + |2\rangle \otimes |1\rangle) + v^2 \cdot |2\rangle \otimes |2\rangle, \end{aligned}$$

$$\begin{aligned} \frac{1}{\sqrt{2}}(|1\rangle \otimes |2\rangle + |2\rangle \otimes |1\rangle) &\mapsto \frac{1}{\sqrt{2}}((u|1\rangle - v|2\rangle) \otimes (v^*|1\rangle + u^*|2\rangle) + (v^*|1\rangle + u^*|2\rangle) \otimes (u|1\rangle - v|2\rangle)) \\ &= \sqrt{2}uv^* \cdot |1\rangle \otimes |1\rangle + (u^*u - v^*v) \cdot \frac{1}{\sqrt{2}}(|1\rangle \otimes |2\rangle + |2\rangle \otimes |1\rangle) - \sqrt{2}vu^* \cdot |2\rangle \otimes |2\rangle, \end{aligned}$$

$$\begin{aligned} |2\rangle \otimes |2\rangle &\mapsto (v^*|1\rangle + u^*|2\rangle) \otimes (v^*|1\rangle + u^*|2\rangle) \\ &= (v^*)^2 \cdot |1\rangle \otimes |1\rangle + \sqrt{2}v^*u^* \cdot \frac{1}{\sqrt{2}}(|1\rangle \otimes |2\rangle + |2\rangle \otimes |1\rangle) + (u^*)^2 \cdot |2\rangle \otimes |2\rangle. \end{aligned}$$

This can be written as, $(|n_1 = 2, n_2 = 0\rangle, |n_1 = 1, n_2 = 1\rangle, |n_1 = 0, n_2 = 2\rangle)$

$$\mapsto (|n_1 = 2, n_2 = 0\rangle, |n_1 = 1, n_2 = 1\rangle, |n_1 = 0, n_2 = 2\rangle) \cdot \begin{pmatrix} u^2 & \sqrt{2}uv^* & (v^*)^2 \\ -\sqrt{2}uv & (u^*u - v^*v) & \sqrt{2}v^*u^* \\ v^2 & -\sqrt{2}vu^* & (u^*)^2 \end{pmatrix}.$$

One can check that the 3×3 matrix (\dots) is unitary by brute-force computation,

$$(\dots)^\dagger \cdot (\dots) = (|u|^2 + |v|^2)^2 \cdot \mathbb{1}_{3 \times 3} = \mathbb{1}_{3 \times 3}.$$

(d) represent the basis in (a) by creation operators,

$$|n_1 = 2, n_2 = 0\rangle = \frac{1}{\sqrt{2}}(\hat{b}_1^\dagger)^2|\text{vac}\rangle,$$

$$|n_1 = 1, n_2 = 1\rangle = \hat{b}_1^\dagger \hat{b}_2^\dagger |\text{vac}\rangle,$$

$$|n_1 = 0, n_2 = 2\rangle = \frac{1}{\sqrt{2}}(\hat{b}_2^\dagger)^2|\text{vac}\rangle.$$

Then (note that $\hat{b}_1^\dagger \hat{b}_2^\dagger = \hat{b}_2^\dagger \hat{b}_1^\dagger$),

$$\begin{aligned}
\hat{U}|n_1 = 2, n_2 = 0\rangle &= \frac{1}{\sqrt{2}}(\hat{U}\hat{b}_1^\dagger\hat{U}^\dagger)^2\hat{U}|\text{vac}\rangle = \frac{1}{\sqrt{2}}(u\hat{b}_1^\dagger - v\hat{b}_2^\dagger)^2|\text{vac}\rangle \\
&= [u^2 \cdot \frac{1}{\sqrt{2}}(\hat{b}_1^\dagger)^2 - \sqrt{2}uv \cdot \hat{b}_1^\dagger\hat{b}_2^\dagger + v^2 \cdot \frac{1}{\sqrt{2}}(\hat{b}_2^\dagger)^2]|\text{vac}\rangle, \\
\hat{U}|n_1 = 1, n_2 = 1\rangle &= (\hat{U}\hat{b}_1^\dagger\hat{U}^\dagger)(\hat{U}\hat{b}_2^\dagger\hat{U}^\dagger)\hat{U}|\text{vac}\rangle = (u\hat{b}_1^\dagger - v\hat{b}_2^\dagger)(v^*\hat{b}_1^\dagger + u^*\hat{b}_2^\dagger)|\text{vac}\rangle \\
&= [\sqrt{2}uv^* \cdot \frac{1}{\sqrt{2}}(\hat{b}_1^\dagger)^2 + (uu^* - vv^*) \cdot \hat{b}_1^\dagger\hat{b}_2^\dagger - \sqrt{2}vu^* \cdot \frac{1}{\sqrt{2}}(\hat{b}_2^\dagger)^2]|\text{vac}\rangle, \\
\hat{U}|n_1 = 0, n_2 = 2\rangle &= \frac{1}{\sqrt{2}}(\hat{U}\hat{b}_2^\dagger\hat{U}^\dagger)^2\hat{U}|\text{vac}\rangle = \frac{1}{\sqrt{2}}(v^*\hat{b}_1^\dagger + u^*\hat{b}_2^\dagger)^2|\text{vac}\rangle \\
&= [(v^*)^2 \cdot \frac{1}{\sqrt{2}}(\hat{b}_1^\dagger)^2 + \sqrt{2}v^*u^* \cdot \hat{b}_1^\dagger\hat{b}_2^\dagger + (u^*)^2 \cdot \frac{1}{\sqrt{2}}(\hat{b}_2^\dagger)^2]|\text{vac}\rangle.
\end{aligned}$$

This is consistent with the result of (c).

$$(e) \hat{H} = (\hat{b}_1^\dagger, \hat{b}_2^\dagger) \begin{pmatrix} 0 & t \\ t & 0 \end{pmatrix} \begin{pmatrix} \hat{b}_1 \\ \hat{b}_2 \end{pmatrix}.$$

The 2×2 matrix in the middle is $t\sigma_1$, with eigenvalues t and $-t$ [c.f. Homework #1 Problem 6.(a)]. $\begin{pmatrix} 0 & t \\ t & 0 \end{pmatrix} = U \cdot \begin{pmatrix} t & 0 \\ 0 & -t \end{pmatrix} \cdot U^\dagger$, where $U = \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \end{pmatrix}$ is a unitary matrix (choice of U is not unique).

Define $(\hat{b}'_1, \hat{b}'_2) = (\hat{b}_1, \hat{b}_2) \cdot U$, namely, $\hat{b}'_1 = \frac{1}{\sqrt{2}}\hat{b}_1 + \frac{1}{\sqrt{2}}\hat{b}_2$, $\hat{b}'_2 = \frac{1}{\sqrt{2}}\hat{b}_1 - \frac{1}{\sqrt{2}}\hat{b}_2$, then $[\hat{b}'_i, \hat{b}'_j] = \delta_{i,j}$, and $\hat{H} = t\hat{b}'_1\hat{b}'_1 - t\hat{b}'_2\hat{b}'_2 = t\hat{n}'_1 - t\hat{n}'_2$. Here $\hat{n}'_i \equiv \hat{b}'_i\hat{b}'_i$ is the boson occupation number operator under the new basis. This basis change does not change the boson vacuum, $\hat{b}'_i|\text{vac}\rangle = 0$.

$\epsilon_1 = t$, $\epsilon_2 = -t$, $\hat{b}'_1 = \frac{1}{\sqrt{2}}\hat{b}_1 + \frac{1}{\sqrt{2}}\hat{b}_2$, $\hat{b}'_2 = \frac{1}{\sqrt{2}}\hat{b}_1 - \frac{1}{\sqrt{2}}\hat{b}_2$. [You may swap $\epsilon_{1,2}$, then $\hat{b}'_{1,2}$ should also be swapped. \hat{b}'_i can be multiplied by independent complex phases.]

The occupation basis states $|n'_1, n'_2\rangle \equiv \frac{1}{\sqrt{(n'_1)!(n'_2)!}}(\hat{b}'_1)^{n'_1}(\hat{b}'_2)^{n'_2}|\text{vac}\rangle$ are normalized eigenstates of \hat{H} , with eigenvalue $\epsilon_1 n'_1 + \epsilon_2 n'_2$.

(f) For notation simplicity, define 2×2 matrix $A = a_1\sigma_1 + a_2\sigma_2 + a_3\sigma_3$, and define $\hat{A} = \sum_{i,j} \hat{b}_i^\dagger A_{i,j} \hat{b}_j$. Then $\hat{U} = \exp(i\hat{A})$. Consider $\hat{U} \cdot \hat{b}_k^\dagger \cdot \hat{U}^\dagger = \exp(i\hat{A}) \cdot \hat{b}_k^\dagger \cdot \exp(-i\hat{A})$. By the Baker-Hausdorff formula, this is, $\hat{b}_k^\dagger + \sum_{n=1}^{\infty} \frac{1}{n!} \underbrace{[i\hat{A}, [i\hat{A}, \dots [i\hat{A}, \hat{b}_k^\dagger] \dots]]}_{n\text{-fold commutator}}$.

Use the identity $[\hat{b}_i^\dagger \hat{b}_j, \hat{b}_k^\dagger] = \delta_{j,k} \hat{b}_i^\dagger$, we have $[i\hat{A}, \hat{b}_k^\dagger] = i \sum_i \hat{b}_i^\dagger A_{i,k}$.

By mathematical induction (steps omitted), $\underbrace{[i\hat{A}, [i\hat{A}, \dots [i\hat{A}, \hat{b}_k^\dagger] \dots]]}_{n\text{-fold commutator}} = i^n \sum_i \hat{b}_i^\dagger (A^n)_{i,k}$.

Here A^n is the n -th power of the matrix A , which is also a 2×2 matrix.

Finally, $\hat{U} \cdot \hat{b}_k^\dagger \cdot \hat{U}^\dagger = \hat{b}_k^\dagger + \sum_{n=1}^{\infty} \frac{1}{n!} i^n \sum_i \hat{b}_i^\dagger (A^n)_{i,k} = \sum_i \hat{b}_i^\dagger [\exp(iA)]_{i,k}$.

Comparing to (d), we should have $\exp(\mathfrak{i}A) = \begin{pmatrix} u & v^* \\ -v & u^* \end{pmatrix}$.

Use the result of Homework #1 Problem 6(b),
 $\exp(\mathfrak{i}A) = \cos(\sqrt{a_1^2 + a_2^2 + a_3^2}) \mathbb{1}_{2 \times 2} + \mathfrak{i} \frac{\sin(\sqrt{a_1^2 + a_2^2 + a_3^2})}{\sqrt{a_1^2 + a_2^2 + a_3^2}} \cdot (a_1 \sigma_1 + a_2 \sigma_2 + a_3 \sigma_3).$

Then $u = \cos(\sqrt{a_1^2 + a_2^2 + a_3^2}) + \mathfrak{i} \frac{\sin(\sqrt{a_1^2 + a_2^2 + a_3^2})}{\sqrt{a_1^2 + a_2^2 + a_3^2}} \cdot a_3,$
 $v = \frac{\sin(\sqrt{a_1^2 + a_2^2 + a_3^2})}{\sqrt{a_1^2 + a_2^2 + a_3^2}} \cdot a_2 - \mathfrak{i} \frac{\sin(\sqrt{a_1^2 + a_2^2 + a_3^2})}{\sqrt{a_1^2 + a_2^2 + a_3^2}} \cdot a_1.$

Conversely,

$$a_1 = -\text{Im}(v) \cdot \frac{\arccos[\text{Re}(u)]}{\sin(\arccos[\text{Re}(u)])}, \quad a_2 = \text{Re}(v) \cdot \frac{\arccos[\text{Re}(u)]}{\sin(\arccos[\text{Re}(u)])}, \quad a_3 = \text{Im}(u) \cdot \frac{\arccos[\text{Re}(u)]}{\sin(\arccos[\text{Re}(u)])}. \quad [\text{Note:}$$

solution of $a_{1,2,3}$ is not unique, ‘arccos’ function is not single-valued.]