

Quantum Mechanics 3 - Homework 4 Solution

Solution to question 1

The Hamiltonian is

$$\hat{H} = \hbar\omega\hat{b}^\dagger\hat{b} + \gamma(\hat{b}^\dagger + \hat{b}). \quad (1)$$

We make the substitutions $\hat{b} = \hat{c} - C\hat{I}$, $\hat{b}^\dagger = \hat{c}^\dagger - C\hat{I}$:

$$\begin{aligned} \hat{H} &= \hbar\omega(\hat{c}^\dagger - C\hat{I})(\hat{c} - C\hat{I}) + \gamma(\hat{c}^\dagger + \hat{c}) - 2\gamma C\hat{I} \\ &= \hbar\omega\hat{c}^\dagger\hat{c} + (\gamma - \hbar\omega C)(\hat{c}^\dagger + \hat{c}) + (\hbar\omega C^2 - 2\gamma C)\hat{I}. \end{aligned} \quad (2)$$

Setting $C = \gamma/\hbar\omega$ yields

$$\hat{H} = \omega\hat{c}^\dagger\hat{c} - \frac{\gamma^2}{\hbar\omega}\hat{I}. \quad (3)$$

It is easy to see that

$$[\hat{b}, \hat{b}^\dagger] = \hat{I} \implies [\hat{c}, \hat{c}^\dagger] = \hat{I} \quad (4)$$

$$[\hat{b}, \hat{b}] = 0 \implies [\hat{c}, \hat{c}] = 0 \quad (5)$$

So we conclude that the eigen-energies are (for $\omega \neq 0$)

$$\boxed{E_n = \hbar\omega n_c - \frac{\gamma^2}{\hbar\omega}, \quad n_c = 0, 1, \dots} \quad (6)$$

The eigen-states are

$$|n_c\rangle = \frac{(\hat{c}^\dagger)^{n_c}}{\sqrt{n_c!}}|0_c\rangle. \quad (7)$$

In order to find $|0_c\rangle$, we calculate

$$\langle n_b|0_c\rangle = \langle 0_b|\frac{(\hat{b})^{n_b}}{\sqrt{n_b!}}|0_c\rangle = \langle 0_b|\frac{(\hat{c} - \frac{\gamma}{\hbar\omega}\hat{I})^{n_b}}{\sqrt{n_b!}}|0_c\rangle = \langle 0_b|0_c\rangle\frac{(-\frac{\gamma}{\hbar\omega})^{n_b}}{\sqrt{n_b!}}. \quad (8)$$

In order for $|0_c\rangle$ to be normalized to 1, we have to demand that

$$1 = \sum_{n_b=0}^{\infty} |\langle n_b|0_c\rangle|^2 = \sum_{n_b=0}^{\infty} |\langle 0_b|0_c\rangle|^2 \frac{(\frac{\gamma}{\hbar\omega})^{2n_b}}{n_b!} = |\langle 0_b|0_c\rangle|^2 \sum_{n_b=0}^{\infty} \frac{(\frac{\gamma}{\hbar\omega})^{2n_b}}{n_b!} = |\langle 0_b|0_c\rangle|^2 e^{\gamma^2/(\hbar\omega)^2}. \quad (9)$$

Therefore, we can choose

$$\langle 0_b|0_c\rangle = e^{-\gamma^2/2(\hbar\omega)^2}. \quad (10)$$

Thus

$$\begin{aligned}
|n_c\rangle &= \sum_{n_b=0}^{\infty} \frac{(\hat{c}^\dagger)^{n_c}}{\sqrt{n_c!}} |n_b\rangle \langle n_b|0_c\rangle = \frac{e^{-\gamma^2/2(\hbar\omega)^2}}{\sqrt{n_c!}} \sum_{n_b=0}^{\infty} \frac{(-\frac{\gamma}{\hbar\omega})^{n_b}}{\sqrt{n_b!}} \left(\hat{b}^\dagger + \frac{\gamma}{\hbar\omega}\hat{I}\right)^{n_c} |n_b\rangle \\
&= \frac{e^{-\gamma^2/2(\hbar\omega)^2}}{\sqrt{n_c!}} \sum_{n_b=0}^{\infty} \sum_{k=0}^{n_c} \binom{n_c}{k} (-1)^{n_b} \frac{(\frac{\gamma}{\hbar\omega})^{n_b+n_c-k}}{\sqrt{n_b!}} (\hat{b}^\dagger)^k |n_b\rangle. \\
&= \frac{e^{-\gamma^2/2(\hbar\omega)^2}}{\sqrt{n_c!}} \sum_{n_b=0}^{\infty} \sum_{k=0}^{n_c} \binom{n_c}{k} (-1)^{n_b} \frac{(\frac{\gamma}{\hbar\omega})^{n_b+n_c-k}}{n_b!} \sqrt{(n_b+k)!} |n_b+k\rangle.
\end{aligned} \tag{11}$$

Next, we consider the Hamiltonian of interacting electrons and bosons.

$$\hat{H} = \sum_i \hbar\omega_i \hat{b}_i^\dagger \hat{b}_i + \sum_j \epsilon_j \hat{a}_j^\dagger \hat{a}_j + \sum_{i,j} \gamma_i \hat{a}_j^\dagger \hat{a}_j (\hat{b}_i^\dagger + \hat{b}_i). \tag{12}$$

We try again the same trick and substitute $\hat{b}_i = \hat{c}_i - \frac{\gamma_i}{\hbar\omega_i}\hat{I}$, $\hat{b}_i^\dagger = \hat{c}_i^\dagger - \frac{\gamma_i}{\hbar\omega_i}\hat{I}$:

$$\hat{H} = \sum_i \hbar\omega_i \hat{c}_i^\dagger \hat{c}_i + \sum_j \epsilon_j \hat{a}_j^\dagger \hat{a}_j + \sum_{i,j} \gamma_i \left(\hat{a}_j^\dagger \hat{a}_j - \frac{\hat{I}}{N}\right) (\hat{c}_i^\dagger + \hat{c}_i) + \sum_{i,j} \frac{\gamma_i^2}{\hbar\omega_i} \left(\frac{\hat{I}}{N} - 2\hat{a}_j^\dagger \hat{a}_j\right), \tag{13}$$

where N is the number of electrons states, and we see that we won't be able to cancel out the $\hat{c}_i^\dagger + \hat{c}_i$ term this time. Instead, let us consider $\hat{b}_i = \hat{c}_i - \frac{\gamma_i}{\hbar\omega_i}\hat{N}_e$, $\hat{b}_i^\dagger = \hat{c}_i^\dagger - \frac{\gamma_i}{\hbar\omega_i}\hat{N}_e$, where $\hat{N}_e = \sum_{j=1}^N \hat{a}_j^\dagger \hat{a}_j$ is the electrons number operator. Now:

$$\begin{aligned}
\hat{H} &= \sum_i \hbar\omega_i \hat{c}_i^\dagger \hat{c}_i + \sum_j \epsilon_j \hat{a}_j^\dagger \hat{a}_j + \sum_{i,j} \gamma_i \left(\hat{a}_j^\dagger \hat{a}_j - \frac{\hat{N}_e}{N}\right) (\hat{c}_i^\dagger + \hat{c}_i) + \sum_{i,j} \frac{\gamma_i^2}{\hbar\omega_i} \left(\frac{\hat{N}_e}{N} - 2\hat{a}_j^\dagger \hat{a}_j\right) \\
&= \sum_i \hbar\omega_i \hat{c}_i^\dagger \hat{c}_i + \sum_j \epsilon_j \hat{a}_j^\dagger \hat{a}_j - \hat{N}_e \sum_i \frac{\gamma_i^2}{\hbar\omega_i},
\end{aligned} \tag{14}$$

and the spectrum is

$$E(\{n_{c,i}\}, \{n_{e,j}\}) = \sum_i \hbar\omega_i n_{c,i} + \sum_j \epsilon_j n_{e,j} - \sum_j n_{e,j} \sum_i \frac{\gamma_i^2}{\hbar\omega_i}, \tag{15}$$

and the eigen-states are $\prod_{i,j} |n_{c,i}\rangle \otimes |n_{e,j}\rangle$, where $|n_{e,j}\rangle$ are electronic states and $|n_{c,i}\rangle$ is defined very similar to the expression given in Eq. (11), but with $n_b \rightarrow n_{b,i}$, $\omega \rightarrow \omega_i$, and $\gamma \rightarrow \gamma_i \hat{N}_e$ (note that the \hat{N}_e operator does not act on any of the $|n_{b,i}\rangle$ states).

Solution to question 2

The thermal energy for fermions and bosons is presented in Fig. 1.

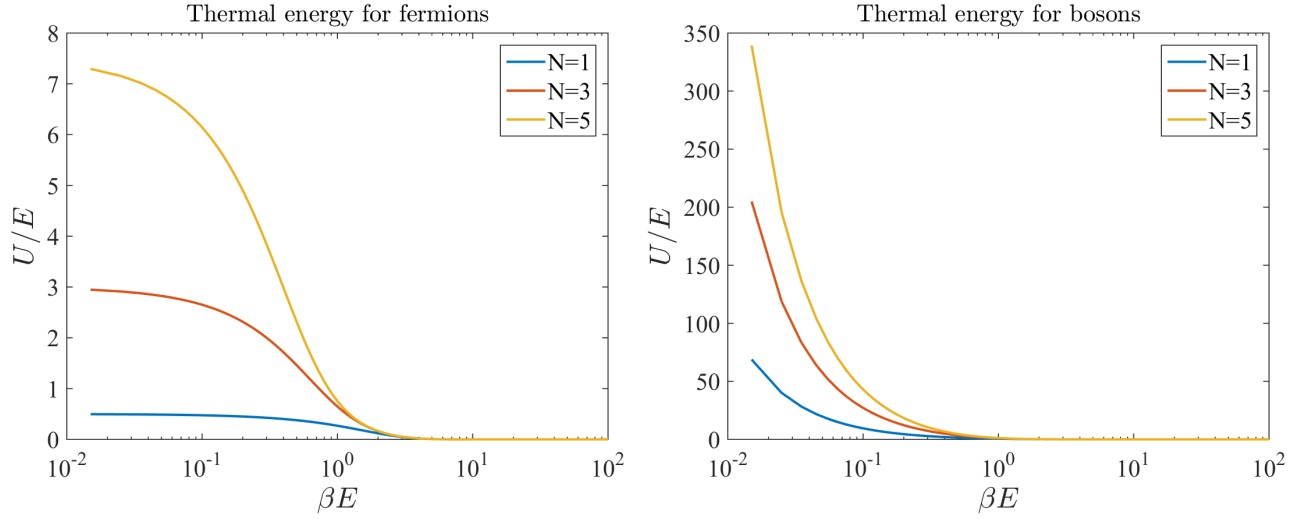


Figure 1: Thermal energy for fermions and bosons.

At cold temperatures ($\beta E \gg 1$) the system is in its ground state. This corresponds to none of the energy levels being occupied and so $U \rightarrow 0$ in this limit (for both fermions and bosons). At hot temperatures ($\beta E \ll 1$) all the states have the same likelihood and so U in this limit is just the arithmetic average of the eigen-energies (with their corresponding degeneracy). Since the matrix ϵ is almost diagonal, the eigen-energies are approximately $1, 2, 3, \dots$ (in units of E). Let's consider fermions first. For $N = 1$, there are only two options: either the state is occupied by a fermion, or not. Therefore

$$\lim_{\beta \rightarrow 0} U(\beta, N = 1) \approx \frac{0 + 1}{2^1} = \frac{1}{2}. \quad (16)$$

For $N = 3$ there are more possibilities as multiple states can be occupied (but never by more than one electron!):

$$\lim_{\beta \rightarrow 0} U(\beta, N = 3) \approx \frac{0 + 1 + 2 + 3 + (1 + 2) + (1 + 3) + (2 + 3) + (1 + 2 + 3)}{2^3} = 3. \quad (17)$$

Similarly, for $N = 5$ (Here I write the energy values along with their degeneracy):

$$\begin{aligned} \lim_{\beta \rightarrow 0} U(\beta, N = 5) &\approx \frac{1}{2^5} [1 \cdot 0 + 1 \cdot 1 + 1 \cdot 2 + 2 \cdot 3 + 2 \cdot 4 + 3 \cdot 5 \\ &\quad + 3 \cdot 6 + 3 \cdot 7 + 3 \cdot 8 + 3 \cdot 9 + 3 \cdot 10 + 2 \cdot 11 + 2 \cdot 12 + 1 \cdot 13 + 1 \cdot 14 + 1 \cdot 15] \\ &= \frac{240}{32} = 7.5 \end{aligned} \quad (18)$$

On the other hand, for bosons, there is an infinite amount of possibilities (even for $N = 1$) since many bosons can occupy the same state. Thus, for bosons $U(\beta \rightarrow 0) \rightarrow \infty$. This divergence is quicker when there are more energy levels (the arithmetic average is greater).

Solution to question 3

We define

$$\hat{\alpha}_{k0} \equiv u_k \hat{c}_{k\uparrow} - v_k \hat{c}_{-k\downarrow}^\dagger \quad (19)$$

$$\alpha_{k1}^\dagger \equiv u_k \hat{c}_{-k\downarrow}^\dagger + v_k \hat{c}_{k\uparrow}, \quad (20)$$

where $u_k, v_k \in \mathbb{R}$, and we require the anti-commutation relations

$$\{\hat{\alpha}_{ki}, \hat{\alpha}_{k'j}^\dagger\} = \delta_{kk'} \delta_{ij} \quad (21)$$

$$\{\hat{\alpha}_{ki}, \hat{\alpha}_{k'j}\} = \{\hat{\alpha}_{ki}^\dagger, \hat{\alpha}_{k'j}^\dagger\} = 0. \quad (22)$$

The requirement of Eq. (21) leads to $u_k^2 + v_k^2 = 1$. For example, for $i = j = 0$:

$$\begin{aligned} 1 &\stackrel{!}{=} \{\hat{\alpha}_{k0}, \hat{\alpha}_{k'0}^\dagger\} = \{u_k \hat{c}_{k\uparrow} - v_k \hat{c}_{-k\downarrow}^\dagger, u_k \hat{c}_{k'\uparrow} - v_k \hat{c}_{-k'\downarrow}^\dagger\} \\ &= u_k^2 \underbrace{\{\hat{c}_{k\uparrow}^\dagger, \hat{c}_{k\uparrow}\}}_1 - u_k v_k \underbrace{\{\hat{c}_{k\uparrow}^\dagger, \hat{c}_{-k\downarrow}\}}_0 - u_k v_k \underbrace{\{\hat{c}_{-k\downarrow}, \hat{c}_{k\uparrow}^\dagger\}}_0 + v_k^2 \underbrace{\{\hat{c}_{-k\downarrow}, \hat{c}_{-k\downarrow}^\dagger\}}_1 \\ &= u_k^2 + v_k^2. \end{aligned} \quad (23)$$

In a similar manner, it can be shown that Eq. (21) holds for other values of i, j only if $u_k^2 + v_k^2 = 1$. Eq. (22) is automatically satisfied due to the construction of $\hat{\alpha}_{k0}$ and $\hat{\alpha}_{k1}^\dagger$ in Eqs. (19) and (20). The inverse relations are given by

$$\hat{c}_{k\uparrow} = u_k \hat{\alpha}_{k0} + v_k \hat{\alpha}_{k1}^\dagger \quad (24)$$

$$\hat{c}_{-k\downarrow}^\dagger = u_k \hat{\alpha}_{k1}^\dagger - v_k \hat{\alpha}_{k0}. \quad (25)$$

We focus first on the free Hamiltonian, which can be expressed as

$$\hat{H}_0 = \sum_k \xi_k \left(\hat{c}_{k,\uparrow}^\dagger \hat{c}_{k,\uparrow} + \hat{c}_{-k,\downarrow}^\dagger \hat{c}_{-k,\downarrow} \right). \quad (26)$$

We now calculate the expression in the parenthesis in terms of $\alpha_{k0}, \alpha_{k1}^\dagger$.

$$\begin{aligned} \hat{c}_{k,\uparrow}^\dagger \hat{c}_{k,\uparrow} + \hat{c}_{-k,\downarrow}^\dagger \hat{c}_{-k,\downarrow} &= (u_k \hat{\alpha}_{k0}^\dagger + v_k \hat{\alpha}_{k1}) (u_k \hat{\alpha}_{k0} + v_k \hat{\alpha}_{k1}^\dagger) + (u_k \hat{\alpha}_{k1}^\dagger - v_k \hat{\alpha}_{k0}) (u_k \hat{\alpha}_{k1} - v_k \hat{\alpha}_{k0}^\dagger) \\ &= u_k^2 (\hat{\alpha}_{k0}^\dagger \hat{\alpha}_{k0} + \hat{\alpha}_{k1}^\dagger \hat{\alpha}_{k1}) + u_k v_k (\hat{\alpha}_{k0}^\dagger \hat{\alpha}_{k1}^\dagger - \hat{\alpha}_{k1}^\dagger \hat{\alpha}_{k0}^\dagger) \\ &\quad + u_k v_k (\hat{\alpha}_{k1} \hat{\alpha}_{k0} - \hat{\alpha}_{k0} \hat{\alpha}_{k1}) + v_k^2 (\hat{\alpha}_{k1} \hat{\alpha}_{k1}^\dagger + \hat{\alpha}_{k0} \hat{\alpha}_{k0}^\dagger) \\ &= (u_k^2 - v_k^2) (\hat{\alpha}_{k0}^\dagger \hat{\alpha}_{k0} + \hat{\alpha}_{k1}^\dagger \hat{\alpha}_{k1}) + 2u_k v_k \hat{\alpha}_{k0}^\dagger \hat{\alpha}_{k1}^\dagger + 2u_k v_k \hat{\alpha}_{k1} \hat{\alpha}_{k0} + v_k^2, \end{aligned} \quad (27)$$

where the last step is due to the anti-commutation relations of Eqs. (21) and (22). We now move to the interaction term in the Hamiltonian. We calculate

$$\begin{aligned} \hat{c}_{k,\uparrow}^\dagger \hat{c}_{-k,\downarrow}^\dagger &= (u_k \hat{\alpha}_{k0}^\dagger + v_k \hat{\alpha}_{k1}) (u_k \hat{\alpha}_{k1}^\dagger - v_k \hat{\alpha}_{k0}) = u_k^2 \hat{\alpha}_{k0}^\dagger \hat{\alpha}_{k1}^\dagger + u_k v_k (-\hat{\alpha}_{k0}^\dagger \hat{\alpha}_{k0} + \hat{\alpha}_{k1} \hat{\alpha}_{k1}^\dagger) - v_k^2 \hat{\alpha}_{k1} \hat{\alpha}_{k0} \\ &= u_k^2 \hat{\alpha}_{k0}^\dagger \hat{\alpha}_{k1}^\dagger - u_k v_k (\hat{\alpha}_{k0}^\dagger \hat{\alpha}_{k0} + \hat{\alpha}_{k1} \hat{\alpha}_{k1}) - v_k^2 \hat{\alpha}_{k1} \hat{\alpha}_{k0} + u_k v_k. \end{aligned} \quad (28)$$

Also,

$$\hat{c}_{-k,\downarrow} \hat{c}_{k,\uparrow} = \left(\hat{c}_{k,\uparrow}^\dagger \hat{c}_{-k,\downarrow}^\dagger \right)^\dagger = u_k^2 \hat{\alpha}_{k1} \hat{\alpha}_{k0} - u_k v_k (\hat{\alpha}_{k0}^\dagger \hat{\alpha}_{k0} + \hat{\alpha}_{k1}^\dagger \hat{\alpha}_{k1}) - v_k^2 \hat{\alpha}_{k0}^\dagger \hat{\alpha}_{k1}^\dagger + u_k v_k. \quad (29)$$

We now plug everything (Eq. 27, 28, 29) in the Hamiltonian.

$$\begin{aligned}\hat{H} &= \sum_k \left\{ \left[\xi_k (u_k^2 - v_k^2) + \Delta_k u_k v_k + \Delta_k^* u_k v_k \right] (\hat{\alpha}_{k0}^\dagger \hat{\alpha}_{k0} + \hat{\alpha}_{k1}^\dagger \hat{\alpha}_{k1}) \right. \\ &\quad + \left[2\xi_k u_k v_k - \Delta_k u_k^2 + \Delta_k^* v_k^2 \right] \hat{\alpha}_{k0}^\dagger \hat{\alpha}_{k1}^\dagger + \left[2\xi_k u_k v_k - \Delta_k^* u_k^2 + \Delta_k v_k^2 \right] \hat{\alpha}_{k1} \hat{\alpha}_{k0} \\ &\quad \left. + \xi_k v_k^2 - \Delta_k u_k v_k - \Delta_k^* u_k v_k \right\}.\end{aligned}\quad (30)$$

The third line in Eq. (30) is just a bunch of scalars in Hilbert space, which have no physical importance and therefore can be omitted in the rest of the calculation. In order to make this Hamiltonian diagonalized we need to require that the second line vanishes. Thus, we require

$$2\xi_k u_k v_k - \Delta_k u_k^2 + \Delta_k^* v_k^2 = 0, \quad (31)$$

or (by multiplying Eq. (31) by Δ_k/u_k^2)

$$\frac{\Delta_k^*}{\Delta_k} \Delta_k^2 \frac{v_k^2}{u_k^2} + 2\xi_k \Delta_k \frac{v_k}{u_k} - \Delta_k^2 = 0. \quad (32)$$

Defining $x \equiv \Delta_k v_k / u_k$, we get a quadratic equation for x ,

$$\frac{\Delta_k^*}{\Delta_k} x^2 + 2\xi_k x - \Delta_k^2 = 0. \quad (33)$$

The solution for x is¹

$$\Delta_k \frac{v_k}{u_k} = x = \left(-\xi_k + \sqrt{\xi_k^2 + |\Delta_k|^2} \right) \frac{\Delta_k}{\Delta_k^*} = (-\xi_k + E_k) e^{2i\phi_k}, \quad (34)$$

where $E_k \equiv \sqrt{\xi_k^2 + |\Delta_k|^2}$ and $\phi_k \equiv \arg \Delta_k$.

We have two equations with two unknowns:

$$u_k^2 + v_k^2 = 1 \quad (35)$$

$$|\Delta_k| \frac{v_k}{u_k} = -\xi_k + E_k. \quad (36)$$

The solutions for these equations are

$$u_k^2 = \frac{|\Delta_k|^2}{|\Delta_k|^2 + (E_k - \xi_k)^2} = \frac{E_k^2 - \xi_k^2}{E_k^2 - \xi_k^2 + (E_k - \xi_k)^2} = \frac{E_k + \xi_k}{E_k + \xi_k + (E_k - \xi_k)} = \frac{1}{2} + \frac{\xi_k}{2E_k} \quad (37)$$

$$v_k^2 = \frac{(E_k - \xi_k)^2}{|\Delta_k|^2 + (E_k - \xi_k)^2} = \frac{(E_k - \xi_k)^2}{E_k^2 - \xi_k^2 + (E_k - \xi_k)^2} = \frac{E_k - \xi_k}{E_k + \xi_k + (E_k - \xi_k)} = \frac{1}{2} - \frac{\xi_k}{2E_k} \quad (38)$$

¹We rule out the "–" solution. This is because for that solution, $\Delta_k = 0$ would then imply $\xi_k = 0$, which is not true for all k values.

Knowing the expressions for u and v , we can now calculate

$$\xi_k (u_k^2 - v_k^2) = \frac{\xi_k^2}{E_k} \quad (39)$$

$$\begin{aligned} \Delta_k u_k v_k + \Delta_k^* u_k v_k &= 2 \operatorname{Re}(\Delta_k^* u_k v_k) = 2u_k^2 \operatorname{Re}\left(\frac{\Delta_k^*}{\Delta_k} \Delta_k \frac{v_k}{u_k}\right) \stackrel{(1)}{=} 2u_k^2 \operatorname{Re}(E_k - \xi_k) \\ &= 2u_k^2 (E_k - \xi_k) = \left(1 + \frac{\xi_k}{E_k}\right) (E_k - \xi_k) = \frac{E_k^2 - \xi_k^2}{E_k}, \end{aligned} \quad (40)$$

where equality (1) follows from Eq. (34). Finally, we plug Eqs. (39) and (40) back in the Hamiltonian of Eq. (30) to find

$$\hat{H} = \sum_k E_k \left(\hat{\alpha}_{k0}^\dagger \hat{\alpha}_{k0} + \hat{\alpha}_{k1}^\dagger \hat{\alpha}_{k1} \right), \quad E_k \equiv \sqrt{\xi_k^2 + |\Delta_k|^2}. \quad (41)$$

Solution to question 4

Solution to item 1

On the one hand, we have

$$\begin{aligned} \hat{\eta}_k \hat{H} |n_1, n_2, \dots, n_k, \dots\rangle &= \hat{\eta}_k \left(\sum_{m=1}^N \Lambda_m n_m + E_0 \right) |n_1, n_2, \dots, n_k, \dots\rangle \\ &= \left(\sum_{m=1}^N \Lambda_m n_m + E_0 \right) \sqrt{n_k} |n_1, n_2, \dots, n_k - 1, \dots\rangle \end{aligned} \quad (42)$$

$$\begin{aligned} \hat{H} \hat{\eta}_k |n_1, n_2, \dots, n_k, \dots\rangle &= \hat{H} \sqrt{n_k} |n_1, n_2, \dots, n_k - 1, \dots\rangle \\ &= \sqrt{n_k} \left(\sum_{m=1}^N \Lambda_m n_m - \Lambda_k + E_0 \right) |n_1, n_2, \dots, n_k - 1, \dots\rangle, \end{aligned} \quad (43)$$

and thus

$$\left[\hat{\eta}_k, \hat{H} \right] |n_1, n_2, \dots, n_k, \dots\rangle = \sqrt{n_k} \Lambda_k |n_1, n_2, \dots, n_k - 1, \dots\rangle. \quad (44)$$

On the other hand

$$\Lambda_k \hat{\eta}_k |n_1, n_2, \dots, n_k, \dots\rangle = \Lambda_k \sqrt{n_k} |n_1, n_2, \dots, n_k - 1, \dots\rangle, \quad (45)$$

and therefore

$$\left(\left[\hat{\eta}_k, \hat{H} \right] - \Lambda_k \hat{\eta}_k \right) |n_1, n_2, \dots, n_k, \dots\rangle = 0. \quad (46)$$

This is true for every state in Fock space and thus we conclude

$$\left[\hat{\eta}_k, \hat{H} \right] - \Lambda_k \hat{\eta}_k = 0. \quad (47)$$

Solution to item 2

We compute

$$\begin{aligned}
[\hat{\eta}_k, \hat{H}] &= \left[\sum_{l=1}^N (g_{kl}\hat{c}_l + h_{kl}\hat{c}_l^\dagger), \sum_{i,j=1}^N \left[\hat{c}_i^\dagger A_{ij}\hat{c}_j + \frac{1}{2} (\hat{c}_i^\dagger B_{ij}\hat{c}_j^\dagger + \text{h.c.}) \right] \right] \\
&= \sum_{l=1}^N \sum_{i,j=1}^N g_{kl} A_{ij} [\hat{c}_l, \hat{c}_i^\dagger \hat{c}_j] + \sum_{l=1}^N \sum_{i,j=1}^N h_{kl} A_{ij} [\hat{c}_l^\dagger, \hat{c}_i^\dagger \hat{c}_j] + \frac{1}{2} \sum_{l=1}^N \sum_{i,j=1}^N g_{kl} B_{ij} [\hat{c}_l, \hat{c}_i^\dagger \hat{c}_j^\dagger] \\
&\quad + \frac{1}{2} \sum_{l=1}^N \sum_{i,j=1}^N h_{kl} B_{ij} [\hat{c}_l^\dagger, \hat{c}_i^\dagger \hat{c}_j^\dagger] + \frac{1}{2} \sum_{l=1}^N \sum_{i,j=1}^N g_{kl} B_{ij} [\hat{c}_l, \hat{c}_j \hat{c}_i] + \frac{1}{2} \sum_{l=1}^N \sum_{i,j=1}^N h_{kl} B_{ij} [\hat{c}_l^\dagger, \hat{c}_j \hat{c}_i]. \quad (48)
\end{aligned}$$

We need to evaluate the following commutators,

$$[\hat{c}_l, \hat{c}_i^\dagger \hat{c}_j] = \hat{c}_l \hat{c}_i^\dagger \hat{c}_j - \hat{c}_i^\dagger \hat{c}_j \hat{c}_l = \hat{c}_l \hat{c}_i^\dagger \hat{c}_j + (\delta_{il} - \hat{c}_l \hat{c}_i^\dagger) \hat{c}_j = \delta_{il} \hat{c}_j \quad (49)$$

$$[\hat{c}_l^\dagger, \hat{c}_i^\dagger \hat{c}_j] = \hat{c}_l^\dagger \hat{c}_i^\dagger \hat{c}_j - \hat{c}_i^\dagger \hat{c}_j \hat{c}_l^\dagger = \hat{c}_l^\dagger \hat{c}_i^\dagger \hat{c}_j - \hat{c}_i^\dagger (\delta_{jl} - \hat{c}_l^\dagger \hat{c}_j) = -\delta_{jl} \hat{c}_i^\dagger \quad (50)$$

$$[\hat{c}_l, \hat{c}_i^\dagger \hat{c}_j^\dagger] = \hat{c}_l \hat{c}_i^\dagger \hat{c}_j^\dagger - \hat{c}_i^\dagger \hat{c}_j^\dagger \hat{c}_l = \hat{c}_l \hat{c}_i^\dagger \hat{c}_j^\dagger - \hat{c}_i^\dagger (\delta_{jl} - \hat{c}_l \hat{c}_j^\dagger) = \hat{c}_l \hat{c}_i^\dagger \hat{c}_j^\dagger + (\delta_{il} - \hat{c}_l \hat{c}_i^\dagger) \hat{c}_j^\dagger - \hat{c}_i^\dagger \delta_{jl} = \delta_{il} \hat{c}_j^\dagger - \delta_{jl} \hat{c}_i^\dagger \quad (51)$$

$$[\hat{c}_l^\dagger, \hat{c}_i^\dagger \hat{c}_j^\dagger] = [\hat{c}_l, \hat{c}_j \hat{c}_i] = 0 \quad (52)$$

$$[\hat{c}_l^\dagger, \hat{c}_j \hat{c}_i] = \hat{c}_l^\dagger \hat{c}_j \hat{c}_i - \hat{c}_j \hat{c}_i \hat{c}_l^\dagger = \hat{c}_l^\dagger \hat{c}_j \hat{c}_i - \hat{c}_j (\delta_{il} - \hat{c}_l^\dagger \hat{c}_i) = \hat{c}_l^\dagger \hat{c}_j \hat{c}_i + (\delta_{jl} - \hat{c}_l^\dagger \hat{c}_j) \hat{c}_i - \hat{c}_j \delta_{il} = \delta_{jl} \hat{c}_i - \delta_{il} \hat{c}_j. \quad (53)$$

Thus

$$\begin{aligned}
[\hat{\eta}_k, \hat{H}] &= \sum_{i,j=1}^N g_{ki} A_{ij} \hat{c}_j - \sum_{i,j=1}^N h_{kj} A_{ij} \hat{c}_i^\dagger + \frac{1}{2} \sum_{i,j=1}^N (g_{ki} B_{ij} \hat{c}_j^\dagger - g_{kj} B_{ij} \hat{c}_i^\dagger) + \frac{1}{2} \sum_{i,j=1}^N (h_{kj} B_{ij} \hat{c}_i - h_{ki} B_{ij} \hat{c}_j) \\
&= \sum_{i,j=1}^N g_{kj} A_{ji} \hat{c}_i - \sum_{i,j=1}^N h_{kj} A_{ij} \hat{c}_i^\dagger + \frac{1}{2} \sum_{i,j=1}^N (g_{kj} B_{ji} \hat{c}_i^\dagger - g_{kj} B_{ij} \hat{c}_i^\dagger) + \frac{1}{2} \sum_{i,j=1}^N (h_{kj} B_{ij} \hat{c}_i - h_{kj} B_{ji} \hat{c}_i) \\
&= \sum_{i,j=1}^N (g_{kj} A_{ji} - h_{kj} B_{ji}) \hat{c}_i + \sum_{i,j=1}^N (g_{kj} B_{ji} - h_{kj} A_{ji}) \hat{c}_i^\dagger. \quad (54)
\end{aligned}$$

Here, in the second line I switched $i \leftrightarrow j$ in some of the terms, while in the last line I used the (anti-)symmetry property of A_{ij} (B_{ij}). We also need

$$\Lambda_k \hat{\eta}_k = \sum_{i=1}^N (\Lambda_k g_{ki} \hat{c}_i + \Lambda_k h_{ki} \hat{c}_i^\dagger). \quad (55)$$

In order to satisfy Eq. (47), we need that the coefficients of each \hat{c}_i^\dagger and \hat{c}_i in Eqs. (54)-(55) to be identical. This implies that

$$\sum_{j=1}^N (g_{kj} A_{ji} - h_{kj} B_{ji}) = \Lambda_k g_{ki} \quad (56)$$

$$\sum_{j=1}^N (g_{kj} B_{ji} - h_{kj} A_{ji}) = \Lambda_k h_{ki}. \quad (57)$$

Solution to item 3

We compute \hat{K}_i^2 :

$$\begin{aligned}\hat{K}_i^2 &= \hat{K}_i \hat{K}_i = \prod_{k=1}^{i-1} (1 - 2\hat{a}_k^\dagger \hat{a}_k) \prod_{j=1}^{i-1} (1 - 2\hat{a}_j^\dagger \hat{a}_j) = \hat{K}_{i-1} \hat{K}_{i-1} (1 - 2\hat{a}_{i-1}^\dagger \hat{a}_{i-1}) (1 - 2\hat{a}_{i-1}^\dagger \hat{a}_{i-1}) \\ &= \hat{K}_{i-1}^2 \left[1 - 4\hat{a}_{i-1}^\dagger \hat{a}_{i-1} + 4(\hat{a}_{i-1}^\dagger \hat{a}_{i-1})^2 \right].\end{aligned}\quad (58)$$

Let us see more closely what is $\hat{a}_{i-1}^\dagger \hat{a}_{i-1}$.

$$\hat{a}_{i-1}^\dagger \hat{a}_{i-1} = \frac{\hat{\sigma}_{i-1}^x + i\hat{\sigma}_{i-1}^y}{2} \frac{\hat{\sigma}_{i-1}^x - i\hat{\sigma}_{i-1}^y}{2} = \frac{1}{4} (\hat{\sigma}_{i-1}^x)^2 + \frac{1}{4} (\hat{\sigma}_{i-1}^y)^2 - \frac{i}{4} [\hat{\sigma}_{i-1}^x, \hat{\sigma}_{i-1}^y] = \frac{1}{2} + \frac{1}{2} \hat{\sigma}_{i-1}^z. \quad (59)$$

Thus

$$\left(\hat{a}_{i-1}^\dagger \hat{a}_{i-1} \right)^2 = \left(\frac{1}{2} + \frac{1}{2} \hat{\sigma}_{i-1}^z \right) \left(\frac{1}{2} + \frac{1}{2} \hat{\sigma}_{i-1}^z \right) = \frac{1}{4} + \frac{1}{4} (\hat{\sigma}_{i-1}^z)^2 + \frac{1}{2} \hat{\sigma}_{i-1}^z = \frac{1}{2} + \frac{1}{2} \hat{\sigma}_{i-1}^z = \hat{a}_{i-1}^\dagger \hat{a}_{i-1}, \quad (60)$$

and so from Eq. (58) we see that

$$\hat{K}_i^2 = \hat{K}_{i-1}^2. \quad (61)$$

Since $\hat{K}_1 \equiv 1$, the solution to this recursion equation is $\hat{K}_i^2 = 1$.

Solution to item 4

I will show here only the proof for Eq. (39) (as the proof for Eq. (40) is very similar).

First, for $i = j$, we have

$$\begin{aligned}\left\{ \hat{c}_i, \hat{c}_i^\dagger \right\} &= \left\{ \hat{K}_i \hat{a}_i, \hat{a}_i^\dagger \hat{K}_i \right\} = \hat{K}_i \hat{a}_i \hat{a}_i^\dagger \hat{K}_i + \hat{a}_i^\dagger \hat{K}_i \hat{K}_i \hat{a}_i \stackrel{(1)}{=} \hat{a}_i \hat{K}_i^2 \hat{a}_i^\dagger + \hat{a}_i^\dagger \hat{K}_i^2 \hat{a}_i \\ &\stackrel{(2)}{=} \hat{a}_i \hat{a}_i^\dagger + \hat{a}_i^\dagger \hat{a}_i = \left\{ \hat{a}_i, \hat{a}_i^\dagger \right\} \stackrel{(3)}{=} 1.\end{aligned}\quad (62)$$

Where in equality (1) I used $[\hat{K}_i, \hat{a}_i] = [\hat{K}_i, \hat{a}_i^\dagger] = 0$, in equality (2) I used $\hat{K}_i^2 = 1$, and equality (3) is due to Eq. (34) (in tutorial 9).

Now, let's see what the anti-commutator yields for $i \neq j$. We will assume without loss of generality that $i > j$. First, note that

$$\hat{K}_i \hat{K}_j = \hat{K}_j \hat{K}_i = \prod_{n=j}^{i-1} (1 - 2\hat{a}_n^\dagger \hat{a}_n) \quad (63)$$

Now we calculate the anti-commutator.

$$\begin{aligned}\left\{ \hat{c}_i, \hat{c}_j^\dagger \right\} &= \left\{ \hat{K}_i \hat{a}_i, \hat{a}_j^\dagger \hat{K}_j \right\} = \hat{K}_i \hat{a}_i \hat{a}_j^\dagger \hat{K}_j + \hat{a}_j^\dagger \hat{K}_j \hat{K}_i \hat{a}_i \stackrel{(1)}{=} \hat{K}_i \hat{K}_j \hat{a}_i \hat{a}_j^\dagger + \hat{K}_j \hat{K}_i \hat{a}_j^\dagger \hat{a}_i + \hat{K}_j [\hat{a}_j^\dagger, \hat{K}_i] \hat{a}_i \\ &\stackrel{(2)}{=} 2\hat{K}_i \hat{K}_j \hat{a}_i \hat{a}_j^\dagger + \hat{K}_j [\hat{a}_j^\dagger, \hat{K}_i] \hat{a}_i,\end{aligned}\quad (64)$$

where in equality (1) I used $[\hat{K}_j, \hat{a}_i] = [\hat{K}_j, \hat{a}_i^\dagger] = 0$ (which is true because $i > j$), and in equality (2) I used $\hat{K}_i \hat{K}_j = \hat{K}_j \hat{K}_i$ and $[\hat{a}_i, \hat{a}_j^\dagger] = 0$. Unlike $[\hat{a}_i^\dagger, \hat{K}_j]$, the commutator $[\hat{a}_j^\dagger, \hat{K}_i]$ does not vanish because

$$\begin{aligned}[\hat{a}_j^\dagger, \hat{K}_i] &= \left[\hat{a}_j^\dagger, \prod_{n=1}^{i-1} (1 - 2\hat{a}_n^\dagger \hat{a}_n) \right] = \prod_{n=1}^{j-1} (1 - 2\hat{a}_n^\dagger \hat{a}_n) \prod_{n=j}^{i-1} (1 - 2\hat{a}_n^\dagger \hat{a}_n) [\hat{a}_j^\dagger, 1 - 2\hat{a}_j^\dagger \hat{a}_j] \\ &= -2\hat{K}_j \cdot \hat{K}_j \hat{K}_i \hat{a}_j^\dagger [\hat{a}_j^\dagger, \hat{a}_j] = -2\hat{K}_i \hat{a}_j^\dagger \left(\left\{ \hat{a}_j^\dagger, \hat{a}_j \right\} - 2\hat{a}_j^\dagger \hat{a}_j \right) = -2\hat{K}_i \hat{a}_j^\dagger (1 - 2\hat{a}_j^\dagger \hat{a}_j). \quad (65)\end{aligned}$$

Therefore

$$\begin{aligned}
\{\hat{c}_i, \hat{c}_j^\dagger\} &= 2\hat{K}_i\hat{K}_j\hat{a}_i\hat{a}_j^\dagger + \hat{K}_j \left[-2\hat{K}_i\hat{a}_j^\dagger (1 - 2\hat{a}_j^\dagger\hat{a}_j) \right] \hat{a}_i \\
&= \left(2\hat{K}_i\hat{K}_j\hat{a}_i\hat{a}_j^\dagger - 2\hat{K}_j\hat{K}_i\hat{a}_j^\dagger\hat{a}_i \right) + 4\hat{K}_i\hat{K}_j \left(\hat{a}_j^\dagger \right)^2 \hat{a}_j\hat{a}_i = 0,
\end{aligned} \tag{66}$$

where the last equality follows from $\hat{K}_i\hat{K}_j = \hat{K}_j\hat{K}_i$, $[\hat{a}_i, \hat{a}_j^\dagger] = 0$ and $(\hat{a}_j^\dagger)^2 = 0$.