1. **Fermion creation and annihilation opertators**
The second quantization for fermions is based on the operator a and its hermitian conjugate $a^\dagger$. The only requirements on them are the anticommutator rules ($\{A, B\} = AB + BA$)

$$\{a, a^\dagger\} = 1, \quad \{a, a\} = \{a^\dagger, a^\dagger\} = 0. \tag{1}$$

(i) Show that $a^\dagger a^\dagger = aa = 0$.

(ii) Prove the relation $a^\dagger a(1 - a^\dagger a) = 0$, which implies that the eigenvalues of the operator $a^\dagger a$ must be 0 and 1. Let $|0\rangle$ and $|1\rangle$ denote the eigenstates.

(iii) Prove the relations $[a^\dagger a, a] = -a$ and $[a^\dagger a, a^\dagger] = a^\dagger$. Applying these on $|0\rangle$ and $|1\rangle$, show that (with appropriate definitions of phases)

$$a^\dagger |0\rangle = |1\rangle, \quad a |1\rangle = |0\rangle, \quad a^\dagger |1\rangle = 0, \quad a |0\rangle = 0. \tag{2}$$

Note the important difference between 0 and $|0\rangle$.

Solution:

(i)

$$\begin{aligned} \{a, a\} = \{a^\dagger, a^\dagger\} &= 0 \\ aa + aa = a^\dagger a^\dagger + a^\dagger a^\dagger &= 0 \\ 2aa = 2a^\dagger a^\dagger &= 0 \\ aa = a^\dagger a^\dagger &= 0 \end{aligned}$$

(ii)

$$\begin{aligned} \{a, a^\dagger\} &= 1 \\ aa^\dagger + a^\dagger a &= 1 \\ a^\dagger a(aa^\dagger + a^\dagger a) &= a^\dagger a \\ a^\dagger \underbrace{aa}_{=0} a^\dagger + a^\dagger a a^\dagger a &= a^\dagger a \\ 0 &= a^\dagger a(1 - a^\dagger a) \end{aligned}$$

Let us assume that the vector $|n\rangle$ is an eigenvector of the operator $a^\dagger a$ with eigenvalue n, meaning that $a^\dagger a |n\rangle = n |n\rangle$. But we do not know the possible values of n yet. Let us now operate by operator $a^\dagger a(1 - a^\dagger a)$ on the vector $|n\rangle$:

$$a^\dagger a(1 - a^\dagger a) |n\rangle = (n - n^2) |n\rangle = n(1 - n) |n\rangle .$$

On the other hand we know that $a^\dagger a(1 - a^\dagger a)\,|n\rangle = 0\,|n\rangle$. Based on these two relations we deduce that

$$n(1-n) = 0 \qquad \rightarrow \qquad n = 0, 1.$$

So the only eigenvectors of $a^\dagger a$ are $|0\rangle$ and $|1\rangle$, with eigenvalues 0 and 1, respectively: $a^\dagger a\,|0\rangle = 0 \cdot |0\rangle$ and $a^\dagger a\,|1\rangle = 1 \cdot |1\rangle$. Let us normalize the vectors so that $\langle 0|0\rangle = \langle 1|1\rangle = 1$. If we furthermore assume that a and $a^\dagger$ are Hermitian conjugates [call this assumption $(*)$], then $a^\dagger a$ is Hermitian, and $|0\rangle$ and $|1\rangle$ are orthogonal: $\langle 0|1\rangle = \langle 0|1|1\rangle = \langle 0|a^\dagger a|1\rangle = \langle 0|0|1\rangle = 0$.

(iii) Here we need the relations $a^\dagger a = 1 - aa^\dagger$ and $aa^\dagger = 1 - a^\dagger a$, deduced from the anticommutator rules. Using them:

$$[a^\dagger a, a] = a^\dagger \underbrace{aa}_{=0} - aa^\dagger a = -a(1 - aa^\dagger) = -a + \underbrace{aa}_{=0} a^\dagger = -a$$

$$[a^\dagger a, a^\dagger] = a^\dagger aa^\dagger - \underbrace{a^\dagger a^\dagger}_{=0} a = a^\dagger(1 - a^\dagger a) = a^\dagger.$$

Let us apply the left-hand side of the first of these on the vector $|n\rangle$. By using $a^\dagger a\,|n\rangle = n\,|n\rangle$, we can write $[a^\dagger a, a]\,|n\rangle = (a^\dagger aa - aa^\dagger a)\,|n\rangle = (a^\dagger aa - an)\,|n\rangle = (a^\dagger a - n)a\,|n\rangle$. This must equal $-a\,|n\rangle$. Rearranging, and then doing the same with the second commutator relation we find

$$a^\dagger a(a\,|n\rangle) = (n-1)(a\,|n\rangle)$$
$$a^\dagger a(a^\dagger\,|n\rangle) = (n+1)(a^\dagger\,|n\rangle).$$

All the four results follow from these by considering the cases $n = 0, 1$.

(1) We do not know a priori what the vector $a^\dagger\,|0\rangle$ is, but the above relations allow us to "test" it by operating with $a^\dagger a$. We see that $a^\dagger a(a^\dagger\,|0\rangle) = 1 \cdot a^\dagger\,|0\rangle$. Therefore $a^\dagger\,|0\rangle$ is an eigenvector of $a^\dagger a$ with eigenvalue 1. Thus we may write $a^\dagger\,|0\rangle = c\,|1\rangle$, where c is an arbitrary complex factor, because $a^\dagger\,|0\rangle$ need not be normalized. In fact $c = 0$ is also possible as far as we know, but invoking assumption $(*)$, we can calculate the norm: $\|a^\dagger\,|0\rangle\|^2 = \langle 0|aa^\dagger|0\rangle = \langle 0|(1 - a^\dagger a)|0\rangle = 1 - 0 = 1$. Thus $|c| = 1$, and we may choose $c = 1$, so that we have $a^\dagger\,|0\rangle = |1\rangle$.

(2) Similarly $a^\dagger a(a\,|1\rangle) = 0$. Thus we conclude that $a\,|1\rangle$ is an eigenvector of $a^\dagger a$ with eigenvalue 0, and therefore $a\,|1\rangle = d\,|0\rangle$. The normalization/phase factor d is now fixed by application of $a^\dagger$, which yields $|1\rangle = da^\dagger\,|0\rangle$. Thus $d = c^{-1} = 1$, and we have $a\,|1\rangle = |0\rangle$, with $\|a\,|1\rangle\|^2 = \langle 0|0\rangle = 1$. Under assumption $(*)$ this normalization would follow directly: $\|a\,|1\rangle\|^2 = \langle 1|a^\dagger a|1\rangle = 1$.

(3,4) The remaining two relations state that $a^\dagger a(a\,|0\rangle) = -1 \cdot (a\,|0\rangle)$ and $a^\dagger a(a^\dagger\,|1\rangle) = 2 \cdot (a^\dagger\,|1\rangle)$, which would appear to imply that $a\,|0\rangle$ and $a^\dagger\,|1\rangle$ are eigenvectors of $a^\dagger a$ with eigenvalues -1 and 2, respectively. However, we know they do not exist, and indeed a direct application of $a^\dagger a^\dagger = aa = 0$ would give $a^\dagger a(a\,|0\rangle) = 0$

and $a^\dagger a(a^\dagger|1\rangle) = (1 - aa^\dagger)(a^\dagger|1\rangle) = 1 \cdot a^\dagger|1\rangle$. These would now imply that $a|0\rangle$ and $a^\dagger|1\rangle$ are eigenvectors of $a^\dagger a$ with eigenvalues 0 and 1, again. This is a contradiction, and so we must have $a|0\rangle = a^\dagger|1\rangle = 0$. A similar conclusion follows by assuming the first two relations [(1),(2)] to hold and then by applying $a^\dagger a^\dagger = aa = 0$: $a^\dagger|1\rangle = a^\dagger a^\dagger|0\rangle = 0$ and $a|0\rangle = aa|1\rangle = 0$. Note also that under the assumption of $(*)$, these would be proved directly by $\|a|0\rangle\|^2 = \langle 0|a^\dagger a|0\rangle = 0$, and $\|a^\dagger|1\rangle\|^2 = \langle 1|aa^\dagger|1\rangle = \langle 1|(1 - a^\dagger a)|1\rangle = 1 - 1 = 0$.

Note: In the original formulation of the problem it was implied that the Hermitian conjugateness of a and $a^\dagger$ $(*)$ need not be assumed, but that it follows from the results $a^\dagger|0\rangle = |1\rangle$, $a|1\rangle = |0\rangle$, $a^\dagger|1\rangle = 0$, and $a|0\rangle = 0$, because then $\langle m|a^\dagger|n\rangle = \langle n|a|m\rangle^*$, with $m, n = 0, 1$. However, this at least requires the result $\langle 0|1\rangle = 0$, which follows trivially only if $a^\dagger a$ is Hermitian. If it is not, then we should actually define separate left and right eigenvectors, which gets complicated! So while the proof may be possible to carry out more generally, it is best to skip it here.

2. **Fermion many-body states**

Consider a fermion system in occupation-number representation, where the basis vectors have the form

$$|n_1, n_2, n_3, ..., n_\infty\rangle\,. \tag{3}$$

Here $1, 2, ...$ label the levels, and $n_1,\ n_2, \ldots$ are their occupations ($= 0$ or 1). Second quantization means simply a new notation, where the approach of the previous exercise is applied to each level separately, i.e. for each level there are separate a_i and $a_i^\dagger$'s. The previous anticommutator rules are generalized trivially:

$$\{a_r, a_s^\dagger\} = \delta_{rs}, \quad \{a_r, a_s\} = \{a_r^\dagger, a_s^\dagger\} = 0. \tag{4}$$

(a) Show that the number operators for states i and j commute: $[a_i^\dagger a_i, a_j^\dagger a_j] = 0$.

Because of the anticommutation of the operators on different levels, one has to be careful in defining the signs in Eq. (3) correctly. One consistent way is to define

$$|n_1, n_2, ..., n_\infty\rangle = (a_1^\dagger)^{n_1}(a_2^\dagger)^{n_2}...(a_\infty^\dagger)^{n_\infty}|0, 0, ..., 0\rangle\,, \tag{5}$$

where the levels always appear in the same (but otherwise arbitrary) order. Correspondingly we write

$$\langle n_1, n_2, ..., n_\infty| = \langle 0, 0, ..., 0|\, a_\infty^{n_\infty} \ldots a_2^{n_1} a_1^{n_1} \tag{6}$$

because $(AB)^\dagger = B^\dagger A^\dagger$. We assume the vacuum states normalized, $\langle 0, 0, \ldots|0, 0, \ldots\rangle = 1$.

(b) Prove that the states $|\{n_k\}\rangle \equiv |n_1, n_1, \ldots, n_\infty\rangle$ are orthonormal: $\langle\{n_k\}|\{n_k'\}\rangle = \delta_{n_1,n_1'}\delta_{n_2,n_2'}\cdots$.

(c) Show that $\langle\{n_k\}|a_i^\dagger a_j|\{n_k\}\rangle = \delta_{ij}n_i$.

(d) Express the state $a_u a_t|0, 0, ..., 1_k, ..., 1_l, ...\rangle$ in a simpler form. Here k and l label two levels and all the occupation numbers not shown are zero.

Solution:

(a) The number operators commute:

$$a_i^\dagger a_i a_j^\dagger a_j = a_i^\dagger(\delta_{ij} - a_j^\dagger a_i)a_j = \delta_{ij}a_i^\dagger a_j - a_i^\dagger a_j^\dagger a_i a_j = \delta_{ij}a_i^\dagger a_j - a_j^\dagger a_i^\dagger a_j a_i$$
$$= \delta_{ij}a_i^\dagger a_j - a_j^\dagger(\delta_{ij} - a_j a_i^\dagger)a_i = a_j^\dagger a_j a_i^\dagger a_i$$

(b) The number states can be proved to be orthonormal for instance as follows. Consider first the case where $\{n_k'\} = \{n_k\}$:

$$\langle\{n_k\}|\{n_k\}\rangle = \langle 0|\cdots a_2^{n_2}a_1^{n_1}(a_1^\dagger)^{n_1}(a_2^\dagger)^{n_2}\cdots|0\rangle = \langle 0|\cdots a_j a_i a_i^\dagger a_j^\dagger\cdots|0\rangle$$

where in the second form only operators where $n_i = 1$ are kept. Then by repeatedly using the anticommutation result $a_i a_i^\dagger = 1 - a_i^\dagger a_i$ and observing that the second term must be zero because $a_i|0\rangle = 0$, the final step yields $\langle\{n_k\}|\{n_k\}\rangle = \langle 0|0\rangle = 1$. The proof that $\langle\{n_k\}|\{n_k'\}\rangle = 0$ when $\{n_k'\} \neq \{n_k\}$ is similar: at some point in the anticommutation process the situation is encountered

$$\langle\{n_k\}|\{n_k'\}\rangle = \langle 0|\cdots a_2^{n_2}a_1^{n_1}(a_1^\dagger)^{n_1'}(a_2^\dagger)^{n_2'}\cdots|0\rangle = \langle 0|\cdots a_j a_i a_k^\dagger a_l^\dagger\cdots|0\rangle$$

where $k \neq i$. Then applying $a_i a_k^\dagger = -a_k^\dagger a_i$ only gives a single term which vanishes because of $a_i|0\rangle = 0$. Hence $\langle\{n_k\}|\{n_k'\}\rangle = \delta_{n_1,n_1'}\delta_{n_2,n_2'}\cdots$.

(c) Using $a_i^\dagger a_i|\{n_k\}\rangle = n_i|\{n_k\}\rangle$ and the normalization $\langle\{n_k\}|\{n_k\}\rangle = 1$, it is now clear that for $i = j$ we have $\langle\{n_k\}|a_i^\dagger a_i|\{n_k\}\rangle = n_i$. For $i \neq j$, $\langle\{n_k\}|a_i^\dagger a_j|\{n_k\}\rangle$ can be shown to vanish for example by considering the four possible cases for the occupation numbers n_i and n_j, which are $(n_i, n_j) = (0,0)$, $(0,1)$, $(1,0)$, $(1,1)$. All cases yield zero either due to $a_j|n_j = 0\rangle = 0$, $a_i^\dagger|n_i = 1\rangle = 0$, or $\langle n_i = 0|a_i^\dagger = 0$. Let us go through the most complicated case (although not very complicated), which is when $n_i = n_j = 1$. Then $a_j|\{n_k\}\rangle = a_j|\ldots n_i = 1\ldots n_j = 1\ldots\rangle = \pm|\ldots n_i = 1\ldots n_j = 0\ldots\rangle$, where the $\pm$-sign is caused by the anticommutation rule. Similarly $\langle\{n_k\}|a_i^\dagger = \langle\ldots n_i = 1\ldots n_j = 1\ldots|a_i^\dagger = \pm\langle\ldots n_i = 0\ldots n_j = 1\ldots|$. Hence $\langle\{n_k\}|a_i^\dagger a_j|\{n_k\}\rangle = \pm\langle\ldots n_i = 0\ldots n_j = 1\ldots|\ldots n_i = 1\ldots n_j = 0\ldots\rangle = 0$, since the number states are orthogonal (see (b)).

Thus $\langle\{n_k\}|a_i^\dagger a_j|\{n_k\}\rangle = n_i\delta_{ij}$.

(d)

$$
\begin{aligned}
& a_u a_t |0,0,\ldots,1_k,\ldots,1_l,\ldots\rangle \\
&= a_u a_t a_k^\dagger a_l^\dagger |vac\rangle \\
&= a_u (\delta_{tk} - a_k^\dagger a_t) a_l^\dagger |vac\rangle \\
&= \delta_{tk} a_u a_l^\dagger |vac\rangle - a_u a_k^\dagger a_t a_l^\dagger |vac\rangle \\
&= \delta_{tk}(\delta_{ul} - a_l^\dagger a_u)|vac\rangle - a_u a_k^\dagger (\delta_{tl} - a_l^\dagger a_t)|vac\rangle \\
&= \delta_{tk}\delta_{ul}|vac\rangle - \delta_{tk} a_l^\dagger \underbrace{a_u|vac\rangle}_{=0} - \delta_{tl} a_u a_k^\dagger |vac\rangle + a_u a_k^\dagger a_l^\dagger \underbrace{a_t|vac\rangle}_{=0} \\
&= \delta_{tk}\delta_{ul}|vac\rangle - \delta_{tl}(\delta_{uk} - a_k^\dagger a_u)|vac\rangle \\
&= \delta_{tk}\delta_{ul}|vac\rangle - \delta_{tl}\delta_{uk}|vac\rangle + \delta_{tl} a_k^\dagger \underbrace{a_u|vac\rangle}_{=0} \\
&= (\delta_{tk}\delta_{ul} - \delta_{tl}\delta_{uk})|vac\rangle
\end{aligned}
$$

3. **Fermion Hamiltonian**
Consider now the usual Hamiltonian in the "first" quantization $H = \sum_{k=1}^{N} T(\boldsymbol{r}_k) + \frac{1}{2}\sum_{k\neq l=1}^{N} V(\boldsymbol{r}_k, \boldsymbol{r}_l)$, where N is the number of particles, $T(\boldsymbol{r}_k) = -\hbar^2\nabla^2_{\boldsymbol{r}_k}/2m$ is the kinetic energy operator and $V(\boldsymbol{r}_k, \boldsymbol{r}_l)$ the interaction potential. In the "second" quantization, this operator transforms to

$$\hat{H} = \sum_{rs} a_r^\dagger T_{rs} a_s + \frac{1}{2}\sum_{rstu} a_r^\dagger a_s^\dagger V_{rs,tu} a_u a_t, \tag{7}$$

where T_{rs} and $V_{rs,tu}$ are the matrix elements of $T(\boldsymbol{r}_k)$ and $V(\boldsymbol{r}_k, \boldsymbol{r}_l)$ (in $V_{rs,tu}$ states t and u are the initial states, and r and t refer to the same particle). Without trying to go through the lengthy and dull derivation of Eq. (7) (see for example, Fetter-Walecka, Quantum Theory of Many-Particle Systems, pages 3-18), use the equations of previous problem to calculate the following matrix elements and interpret the results:

$$
\begin{aligned}
&\langle 0,0,...|\hat{H}|0,0,...\rangle \\
&\langle 0,0,...,1_k,...,1_l,...|\hat{H}|0,0,...\rangle \\
&\langle 0,0,...,1_k,...|\hat{H}|0,0,...,1_l,...\rangle \\
&\langle 0,0,...,1_k,...,1_l,...|\hat{H}|0,0,...,1_k,...,1_l,...\rangle \\
&\langle 0,0,...,1_k,...,1_l,...|\hat{H}|0,0,...,1_v,...,1_w,...\rangle.
\end{aligned}
$$

Here all the occupation numbers not shown are zero, and k, l, v and w refer to different levels. (Notice that the exchange terms are automatically included.)

Solution:
Taking the matrix elements (e.g. $\langle 0,0,...,1_k,...,1_l,...|\hat{H}|0,0,...,1_v,...,1_w,...\rangle$) reduces to the calculation of two different kind of matrix elements:

$$\langle 0,0,...,1_k,...,1_l,...|a_r^\dagger a_s|0,0,...,1_v,...,1_w,...\rangle$$
$$\langle 0,0,...,1_k,...,1_l,...|a_r^\dagger a_s^\dagger a_u a_t|0,0,...,1_v,...,1_w,...\rangle.$$

The main idea is to express kets $|0,0,...,1_v,...,1_w,...\rangle$ and bras $\langle 0,0,...,1_k,...,1_l,...|$ in the form

$$|0,0,...,1_v,...,1_w,...\rangle = a_v^\dagger a_w^\dagger\,|0,\ldots,0,\ldots\rangle = a_v^\dagger a_w^\dagger\,|\mathrm{vac}\rangle$$

and

$$\langle 0,0,...,1_k,...,1_l,...| = \langle 0,\ldots,0,\ldots|\,a_l a_k = \langle \mathrm{vac}|\,a_l a_k$$

[note order of operators: $(AB)^\dagger = B^\dagger A^\dagger$] and then to change the order of the operators so that one may apply $\ldots a_r\,|\mathrm{vac}\rangle = 0$ or $\langle \mathrm{vac}|\,a_s^\dagger \ldots = 0$. The changing of the order of the operators is done by using the anticommutator relation: $\{a_r, a_s^\dagger\} = a_r a_s^\dagger + a_s^\dagger a_r = \delta_{rs}$.

Here is an example with one of the hardest inner products

$$\langle 0,0,...,1_k,...,1_l,...|a_r^\dagger a_s|0,0,...,1_v,...,1_w,...\rangle$$

and all others go similarly:

$$\begin{aligned}
&\langle 0,0,...,1_k,...,1_l,...|a_r^\dagger a_s|0,0,...,1_v,...,1_w,...\rangle \\
&= \langle 0,\ldots,0,\ldots|a_l\ \underbrace{a_k a_r^\dagger}_{\delta_{kr}-a_r^\dagger a_k}\ a_s a_v^\dagger a_w^\dagger|0,\ldots,0,\ldots\rangle \\
&= \delta_{kr}\langle \mathrm{vac}|a_l\ \underbrace{a_s a_v^\dagger}_{\delta_{sv}-a_v^\dagger a_s}\ a_w^\dagger|\mathrm{vac}\rangle - \underbrace{\langle \mathrm{vac}|a_l a_r^\dagger a_k a_s a_v^\dagger a_w^\dagger|\mathrm{vac}\rangle}_{A} \\
&= \delta_{kr}\delta_{sv}\langle \mathrm{vac}|\ \underbrace{a_l a_w^\dagger}_{\delta_{lw}-a_w^\dagger a_l}\ |\mathrm{vac}\rangle - \delta_{kr}\langle \mathrm{vac}|a_l a_v^\dagger a_s a_w^\dagger|\mathrm{vac}\rangle - A \\
&= \delta_{kr}\delta_{sv}\delta_{lw}\underbrace{\langle \mathrm{vac}|\mathrm{vac}\rangle}_{=1} - \underbrace{\langle \mathrm{vac}|a_w^\dagger a_l|\mathrm{vac}\rangle}_{=0} - \delta_{kr}\langle \mathrm{vac}|a_l a_v^\dagger a_s a_w^\dagger|\mathrm{vac}\rangle - A \\
&\ \vdots \\
&= \delta_{kr}\delta_{sv}\delta_{lw} - \delta_{kr}\delta_{sw}\delta_{lv} + \delta_{lr}\delta_{sw}\delta_{kv} - \delta_{lr}\delta_{sv}\delta_{kw}.
\end{aligned}$$

1)
Using the calculation method introduced above we find that

$$\langle 0,0,...|\hat{H}|0,0,...\rangle = \sum_{rs} T_{rs}\cdot 0 + \frac{1}{2}\sum_{rstu} V_{rs,tu}\cdot 0 = 0$$

as is natural. There are no particles in vacuum, so there is no kinetic or interaction energy.

2)
Clearly

$$\langle 0,0,...,1_k,...,1_l,...|\hat{H}|0,0,...\rangle = 0$$

This is natural also, because the initial state $|0,0,\ldots\rangle$ is the vacuum while the final state has two particles in it. One cannot simply excite particles from the vacuum with any "normal" particle-conserving interaction V. (This will be different in the BCS theory of superconductors.)

3)
The single particle at l:th momentum state is the initial state and the single particle at k:th momentum state the final state:

$$\langle 0,0,...,1_k,...|\hat{H}|0,0,...,1_l,...\rangle = T_{kl}$$

Interaction must involve at least two particles, so in the absence of a second one, there is only kinetic energy.

4)
Here it should be noted that only the case $k \neq l$ makes sense, because $k = l$ would correspond to a double occupation of the state. So with that in mind

$$\begin{aligned}&\langle 0,0,...,1_k,...,1_l,...|\hat{H}|0,0,...,1_k,...,1_l,...\rangle \\ &= T_{kk} + T_{ll} + \frac{1}{2}(V_{kl,kl} - V_{lk,kl} - V_{kl,lk} + V_{lk,lk})\end{aligned}$$

This describes the kinetic energy of two particles and the interaction between them, with all possible exchanges of particle enumeration, i.e. the exchange terms. The result is best obtained as a special case of 5 below.

5)
Actually just a more general version of case 4.

$$\begin{aligned}&\langle 0,0,...,1_k,...,1_l,...|\hat{H}|0,0,...,1_v,...,1_w,...\rangle \\ &= T_{kv}\delta_{lw} - T_{kw}\delta_{lv} - T_{lv}\delta_{kw} + T_{lw}\delta_{kv} + \frac{1}{2}(V_{kl,vw} - V_{lk,vw} - V_{kl,wv} + V_{lk,wv})\end{aligned}$$

Again, only $k \neq l$ and $v \neq w$ makes sense, but the result has been written without these restrictions. It is easy to see that the result is zero if $k = l$ or $v = w$. And if $k = v \neq l = w$, then case 4 is reproduced. In the case where $k = w \neq l = v$, the kinetic-energy terms have negative signs. And if $k \neq l \neq v \neq w$, then all the kinetic-energy-terms are zero. (Maybe this was the original idea behind having separate cases 4 and 5, and in this order.)

Note: You may additionally check that these results, obtained here from the second-quantized formalism, can really be derived directly from the first-quantized theory

in cases where particle numbers in the matrix elements are the same on the left and right sides of the matrix elements. Thus if we define for example the two-particle Slater deteminants (we drop spin indices for simplicity, although for fermions they should be there)

$$\Phi^{(2)}_{kl}(\mathbf{r}_1,\mathbf{r}_2) = \frac{1}{\sqrt{2}}[\phi_k(\mathbf{r}_1)\phi_l(\mathbf{r}_2) - \phi_l(\mathbf{r}_1)\phi_k(\mathbf{r}_2)]$$

then, for example, the case 5 above should be obtained as

$$\begin{aligned}\langle k,l|H^{(2)}|v,w\rangle &= \int d^3r_1 \int d^3r_2 [\Phi^{(2)}_{kl}(\mathbf{r}_1,\mathbf{r}_2)]^* H^{(2)}(\mathbf{r}_1,\mathbf{r}_2)\Phi^{(2)}_{vw}(\mathbf{r}_1,\mathbf{r}_2) \\ &= T_{kv}\delta_{lw} - T_{kw}\delta_{lv} - T_{lv}\delta_{kw} + T_{lw}\delta_{kv} + \frac{1}{2}(V_{kl,vw} - V_{lk,vw} - V_{kl,wv} + V_{lk,wv})\end{aligned}$$

Here $H^{(2)}$ is the first-quantized Hamiltonian for a two-particle system and we define $T_{kl} = \int d^3r_1 \phi^*_k(\mathbf{r}_1) T(\mathbf{r}_1)\phi_k(\mathbf{r}_1)$ etc. as in the lecture notes. It is instructive to see how the terms with negative signs are those where the particle indices have been exchanged. Clearly, doing things this way is much messier than in second quantization, especially when the number of particles begins to increase.

4. **Fourier transforms**
When using the "box-normalized" (L-periodic) plane waves $\phi_{\boldsymbol{k}}(\boldsymbol{r}) = (1/\sqrt{L^3})e^{i\boldsymbol{k}\cdot\boldsymbol{r}}$ as a basis, the following definitions for the Fourier transformation and its inverse are convenient:

$$F(\boldsymbol{k}) = \int d^3r e^{-i\boldsymbol{k}\cdot\boldsymbol{r}} f(\boldsymbol{r}), \qquad f(\boldsymbol{r}) = \frac{1}{L^3}\sum_{\boldsymbol{k}} e^{i\boldsymbol{k}\cdot\boldsymbol{r}} F(\boldsymbol{k}).$$

Check by substitution of one into the other that they are consistent with each other if

$$\frac{1}{L^3}\int d^3r e^{\pm i(\boldsymbol{k}-\boldsymbol{k}')\cdot\boldsymbol{r}} = \delta_{\boldsymbol{k},\boldsymbol{k}'}, \qquad \frac{1}{L^3}\sum_{\boldsymbol{k}} e^{\pm i\boldsymbol{k}\cdot(\boldsymbol{r}-\boldsymbol{r}')} = \delta(\boldsymbol{r}-\boldsymbol{r}').$$

These are the "orthonormality" and "completeness" relations. Above, all $\boldsymbol{r}$ integrals are over a cube with sides of length L, and the $\boldsymbol{k}$ sums are over the discrete values $\boldsymbol{k} = \frac{2\pi}{L}(n_x, n_y, n_z)$, where $n_{x,y,z}$ are integers. Calculate the orthonormality integral explicitly at least in the case of one dimension.

Solution:
Let's just subtitute the second one in the first and see:

$$\begin{aligned}\int d^3r e^{-i\mathbf{k}\cdot\mathbf{r}} f(\mathbf{r}) &= \int d^3r e^{-i\mathbf{k}\cdot\mathbf{r}} \frac{1}{L^3}\sum_{\mathbf{q}} e^{i\mathbf{q}\cdot\mathbf{r}} F(\mathbf{q}) \\ &= \sum_{\mathbf{q}} F(\mathbf{q}) \underbrace{\frac{1}{L^3}\int d^3r e^{-i(\mathbf{k}-\mathbf{q})\cdot\mathbf{r}}}_{\delta_{\mathbf{k},\mathbf{q}}} = F(\mathbf{k}),\end{aligned}$$

which is as expected. The same in the other direction:

$$\frac{1}{L^3}\sum_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}}F(\mathbf{k}) = \frac{1}{L^3}\sum_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}}\int d^3r' e^{-i\mathbf{k}\cdot\mathbf{r}'}f(\mathbf{r}')$$
$$= \int d^3r' f(\mathbf{r}')\underbrace{\frac{1}{L^3}\sum_{\mathbf{k}} e^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')}}_{\delta(\mathbf{r}-\mathbf{r}')} = f(\mathbf{r}).$$

Also what it should be. That these relations work in practice is sufficient for us. However, the orthonormality is needed frequently enough that it is good to prove it directly. In one dimension

$$\frac{1}{L}\int_0^L dx e^{i(k-k')x} = \frac{1}{L}\int_0^L dx e^{2\pi i(n-n')x/L} = \int_0^1 ds e^{2\pi i(n-n')s}$$

where n, n' are integers. Clearly, if $n' = n$, then the integral equals one. If $n' \neq n$,

$$\int_0^1 ds e^{2\pi i(n-n')s} = \frac{1}{2\pi i(n-n')}|_0^1 e^{2\pi i(n-n')s} = 0$$

because $e^{2\pi i n} = 1$ for any integer n. (You can also do this by first applying $e^{i\alpha} = \cos\alpha + i\sin\alpha$, if you trust the purely real integrals more.) So

$$\int_0^1 ds e^{2\pi i(n-n')s} = \delta_{n,n'}$$

which can still be recast in terms of k and k'.

Note: The "orthonormality" just means that the functions $\phi_{\mathbf{k}}(\mathbf{r}) = \frac{1}{\sqrt{L^3}}e^{i\mathbf{k}\cdot\mathbf{r}}$ are orthonormal with respect to the inner product $(A, B) = \int d^3r A^*(\mathbf{r})B(\mathbf{r})$:

$$(\phi_{\mathbf{k}}, \phi_{\mathbf{k}'}) = \int d^3r \phi^*_{\mathbf{k}}(\mathbf{r})\phi_{\mathbf{k}'}(\mathbf{r}) = \delta_{\mathbf{k},\mathbf{k}'}.$$

The "completeness" relation, which can be written as

$$\sum_{\mathbf{k}} \phi_{\mathbf{k}}(\mathbf{r})\phi^*_{\mathbf{k}}(\mathbf{r}') = \delta(\mathbf{r}-\mathbf{r}'),$$

just means that any function $f(\mathbf{r})$ can be represented in the basis $\phi_{\mathbf{k}}(\mathbf{r})$ as a series $f(\mathbf{r}) = \sum_{\mathbf{k}} \phi_{\mathbf{k}}(\mathbf{r})F_{\mathbf{k}}$, where the expansion coefficients are $F_{\mathbf{k}} = \int d^3r' \phi^*_{\mathbf{k}}(\mathbf{r}')f(\mathbf{r}')$, as can be seen by multiplying the completeness relation by $f(\mathbf{r}')$ and integrating over $\mathbf{r}'$.