Many-particle systems

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So far in the course, we have mainly considered states of a single particle. In this note, we will introduce techniques to describe quantum systems with many particles. We will first find a suitable basis for expressing quantum states of many particles. We will then formulate operators in this space.

1 Quantum states of many-particle systems

An arbitrary state $|\psi\rangle$ of a single particle in a discrete space can be written as

$$|\psi\rangle = \sum_{k'} c_{k'} |k'\rangle, \tag{1}$$

where the $c_{k'}$ are complex coefficients and the states $|k'\rangle$ form a complete and orthonormal basis, i.e.

$$\langle k'|k''\rangle = \delta_{k',k''}, \qquad 1 = \sum_{k'} |k'\rangle\langle k'|. \tag{2}$$

In this section, we will show how to generalize this to many particles.

1.1 Many-particle states for distinguishable particles

To find out how to generalize this to many particles, let us first consider N non-interacting and distinguishable particles. That they are noninteracting means that the Hamiltonian can be written as

$$H = \sum_{i=1}^{N} H_i, \tag{3}$$

where H_i only acts on particle i. An important example is

$$H_i = -\frac{\hbar^2}{2m_i}\nabla_i^2 + V_i(\mathbf{x}_i), \tag{4}$$

where m_i is the mass of particle i and $V_i(\mathbf{x}_i)$ is the potential energy of particle i when it is at position $\mathbf{x}_i$.

To solve the corresponding time-independent Schrödinger equation

$$H\psi(\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N) = E\psi(\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N) \tag{5}$$

we make the ansatz

$$\psi(\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N) = \psi_1(\mathbf{x}_1)\psi_2(\mathbf{x}_2)\cdots\psi_N(\mathbf{x}_N) \tag{6}$$

and note that (5) is fulfilled when

$$H_i\psi_i(\mathbf{x}_i) = E_i\psi_i(\mathbf{x}_i) \tag{7}$$

and

$$E = \sum_{i=1}^{N} E_i. \tag{8}$$

The many-particle state is hence a product of single-particle states.

Using the ket notation, we write

$$\psi_i(\mathbf{x}_i) = \langle \mathbf{x}_i|\psi_i\rangle, \tag{9}$$

and hence the many-particle state is

$$\begin{aligned}\psi(\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N) &= \langle \mathbf{x}_1|\psi_1\rangle\langle \mathbf{x}_2|\psi_2\rangle \cdots \langle \mathbf{x}_N|\psi_N\rangle \\ &= (\langle \mathbf{x}_1| \otimes \langle \mathbf{x}_2| \otimes \cdots \otimes \langle \mathbf{x}_N|)(|\psi_1\rangle \otimes |\psi_2\rangle \otimes \cdots \otimes |\psi_N\rangle).\end{aligned} \tag{10}$$

For a brief reminder of the cross product $\otimes$ and some of its properties see appendix A. The ket representing the many-particle state is hence

$$|\psi\rangle = |\psi_1\rangle \otimes |\psi_2\rangle \otimes \cdots \otimes |\psi_N\rangle. \tag{11}$$

Writing each of the single-particle states in a single-particle basis $|k_i\rangle$, i.e.

$$|\psi_i\rangle = \sum_{k_i} c_{k_i}^{(i)} |k_i\rangle, \tag{12}$$

we have

$$|\psi\rangle = \sum_{k_1,k_2,\ldots,k_N} c_{k_1}^{(1)} c_{k_2}^{(2)} \cdots c_{k_N}^{(N)} |k_1\rangle \otimes |k_2\rangle \otimes \cdots \otimes |k_N\rangle. \tag{13}$$

Note that

$$\begin{aligned}&(\langle k_1| \otimes \langle k_2| \otimes \cdots \otimes \langle k_n|)\,(|k_1'\rangle \otimes |k_2'\rangle \otimes \cdots \otimes |k_N'\rangle) \\ &\qquad = \langle k_1|k_1'\rangle\langle k_2|k_2'\rangle \cdots \langle k_N|k_N'\rangle = \prod_{i=1}^{N} \delta_{k_i,k_i'},\end{aligned} \tag{14}$$

and

$$\begin{aligned}1 &= \sum_{k_1} |k_1\rangle\langle k_1| \otimes \sum_{k_2} |k_2\rangle\langle k_2| \otimes \ldots \otimes \sum_{k_N} |k_N\rangle\langle k_N| \\ &= \sum_{k_1,k_2,\ldots,k_N} (|k_1\rangle \otimes |k_2\rangle \otimes \ldots |k_N\rangle)\,(\langle k_1| \otimes \langle k_2| \otimes \langle k_N|)\,.\end{aligned} \tag{15}$$

Therefore the single-particle product states

$$|k_1\rangle \otimes |k_2\rangle \otimes \ldots \otimes |k_N\rangle \tag{16}$$

form a complete and orthonormal basis for the Hilbert space of N non-interacting and distinguishable particles.

Interaction

What if the particles interact? In that case, we postulate that the interactions do not change the Hilbert space itself. The states (16) then still form a complete and orthonormal basis, and we can expand the many-particle state as

$$|\psi\rangle = \sum_{k_1,k_2,\ldots,k_N} c_{k_1,k_2,\ldots,k_N} |k_1\rangle \otimes |k_2\rangle \otimes \cdots \otimes |k_N\rangle. \tag{17}$$

For the case of non-interacting particles, the coefficients $c_{k_1,k_2,\ldots,k_N}$ separate into a product of N factors each depending only on a single k_i as in (13), but this is no longer true, when the particles interact. The interacting case is hence much harder. To simplify the notation, we shall in the following write

$$|k_1\rangle \otimes |k_2\rangle \otimes \ldots \otimes |k_N\rangle \equiv |k_1, k_2, \ldots, k_N\rangle. \tag{18}$$

1.2 (Anti-)symmetrized product states

If the considered particles are indistinguishable, we need to ensure that the many-particle wavefunction is symmetrized if the particles are bosons and anti-symmetrized if the particles are fermions. States $|\psi\rangle_\pm$ that are properly (anti-)symmetrized fulfil

$$P_{ij}|\psi\rangle_\pm = \pm|\psi\rangle_\pm, \quad \text{for all } i \text{ and } j, \tag{19}$$

where P_{ij} is the operator that exchanges particles i and j. A product of single-particle states does not generally fulfil this requirement, and we thus need a way to construct a complete basis of suitable states.

Starting from a product state, one can obtain a properly (anti-)symmetrized state by applying the (anti-)symmetrization operator, which is defined as

$$S_N^{(\pm)} = \frac{1}{N!} \sum_{k=1}^{N!} (\pm 1)^{p_k} \mathcal{P}_k. \tag{20}$$

Here, the operator $\mathcal{P}_k$ is the kth element of the permutation group of N particles. The permutation group has $N!$ elements as there are $N!$ ways to rearrange N particles. The way we choose to number the elements of the permutation group is unimportant, but we will usually take $k = 1$ to correspond to the trivial permutation, such that applying $\mathcal{P}_1$ to the input state simply gives the input state. Also, p_k is the number of two-particle exchanges that is needed to get from the input state to the kth permutation. As an example, for two particles in different states, i.e. $k' \neq k''$, we have

$$\mathcal{P}_1|k', k''\rangle = |k', k''\rangle, \quad p_1 = 0, \quad \mathcal{P}_2|k', k''\rangle = |k'', k'\rangle, \quad p_2 = 1, \tag{21}$$

and hence

$$S_2^{(\pm)}|k', k''\rangle = \frac{1}{2}(|k', k''\rangle \pm |k'', k'\rangle). \tag{22}$$

particle 2 particle 1 particle 2 particle 1

The first term on the right hand side says that particle 1 is in the state $|k'\rangle$ and particle two is in the state $|k''\rangle$. The second term instead says that particle one is in the state $|k''\rangle$ and particle two is in the state $|k'\rangle$. Note that the state on the right hand side of (22) is not normalized.

In general, we define

$$|k_1, k_2, \ldots, k_N\rangle_\pm \equiv S_N^{(\pm)} |k_1, k_2, \ldots, k_N\rangle. \tag{23}$$

It is left as an exercise to the reader to show that (23) is indeed (anti-)symmetrized. It is also left as an exercise to the reader to show that the (anti-)symmetrization operator fulfils

$$\left(S_N^{(\pm)}\right)^2 = S_N^{(\pm)}, \qquad \left(S_N^{(\pm)}\right)^\dagger = S_N^{(\pm)}, \qquad S_N^{(+)} S_N^{(-)} = 0. \tag{24}$$

The first two of these relations imply that $S_N^{(\pm)}$ is a projector, and the third relation shows that $S_N^{(+)}$ and $S_N^{(-)}$ project onto orthogonal subspaces.

For the case of distinguishable particles, we postulated that a general quantum state can always be written as a superposition of single-particle product states, even if interactions are present. For each of these product states, we can select the (anti-)symmetrized component by applying $S_N^{(\pm)}$. Given the (anti-)symmetrization requirements for bosons and fermions, it is hence natural to postulate that the most general state of indistinguishable particles is a superposition of (anti-)symmetrized product states. This motivates us to construct an orthonormal basis out of the (anti-)symmetrized product states, which we will do next.

1.3 Fock states

Let us first compute the overlap of an (anti-)symmetrized product state with itself:

$$\begin{aligned}
{}_\pm\langle k_1, \ldots, k_N | k_1, \ldots, k_N\rangle_\pm &= \langle k_1, \ldots, k_N | \left(S_N^{(\pm)}\right)^\dagger S_N^{(\pm)} | k_1, \ldots, k_N\rangle \\
&= \langle k_1, \ldots, k_N | S_N^{(\pm)} | k_1, \ldots, k_N\rangle \\
&= \frac{1}{N!} \sum_{k=1}^{N!} (\pm 1)^{p_k} \langle k_1, \ldots, k_N | \mathcal{P}_k | k_1, \ldots, k_N\rangle.
\end{aligned} \tag{25}$$

If the particles are fermions, all the particles are in different single-particle states, and therefore the only nonzero contribution to the sum is the term that contains the trivial permutation with $p_k = 0$. The overlap is therefore $1/N!$. For bosons, we get a nonzero contribution for all permutations that only exchange particles that are in the same single-particle state. To find the number of such permutations, we need to know how many particles occupy each of the allowed single-particle states for the considered product state. Let us label the allowed single-particle states by k and denote the number of particles in $|k\rangle$ by n_k. For

a given k, there are $n_k!$ permutations of the n_k particles. As permutations can be done independently for each group, the total number of permutations that leave $|k_1, \ldots, k_N\rangle$ unchanged is $\prod_k n_k!$. In conclusion,

$$ {}_\pm\langle k_1, \ldots, k_N | k_1, \ldots, k_N \rangle_\pm = \frac{1}{N!} \prod_k n_k!, \tag{26} $$

where we have utilized that for fermions $n_k! = 1$ for all k. This result tells us which factor to multiply the (anti-)symmetrized product states with to obtain normalized states.

It is also clear from the above computation that ${}_\pm\langle k'_1, \ldots, k'_N | k_1, \ldots, k_N \rangle_\pm$ is zero whenever $\{|k_1\rangle, \ldots, |k_N\rangle\}$ and $\{|k'_1\rangle, \ldots, |k'_N\rangle\}$ do not correspond to the same set of single-particle states. Finally, if $\{|k_1\rangle, \ldots, |k_N\rangle\}$ and $\{|k'_1\rangle, \ldots, |k'_N\rangle\}$ represent the same set of single-particle states, then $|k_1, \ldots, k_N\rangle_\pm$ and $|k'_1, \ldots, k'_N\rangle_\pm$ are equal, except possibly for an overall minus sign in the case of fermions. We hence only need to consider a given set of single-particle states once to get a complete set of basis states. For this reason, it is more convenient to use a notation, where the basis kets are labeled only by the number of particles n_k in each of the single-particle states $|k\rangle$. To resolve the ambiguity of the overall sign in the case of fermions, we decide on a particular order of the single-particle states. The jth single-particle state in this order is denoted k_j, and j runs from one up to the number of different single-particle states, which could be infinite. This leads us to the definition of the Fock state as

$$ |n_{k_1}, n_{k_2}, \ldots\rangle_\pm = C_\pm S_N^\pm | \overbrace{k_1 k_1 k_1 \ldots}^{n_{k_1} \text{ times}} \overbrace{k_2 k_2 k_2 \ldots}^{n_{k_2} \text{ times}} \ldots \rangle, \tag{27} $$

where

$$ C_+ = \sqrt{\frac{N!}{\prod_i n_{k_i}!}}, \qquad C_- = \sqrt{N!}, \qquad N = \sum_i n_{k_i}. \tag{28} $$

Note that the Fock state is defined without a need to number the individual particles. The Fock states are orthonormal

$$ {}_\pm\langle n_{k_1}, n_{k_2}, \ldots | n'_{k_1}, n'_{k_2}, \ldots \rangle_\pm = \prod_i \delta_{n_{k_i}, n'_{k_i}}. \tag{29} $$

It also follows from the postulate made above that the Fock states are complete, and hence we have the completeness relation,

$$ 1 = \sum_{n_{k_1}, n_{k_2}, \ldots} |n_{k_1}, n_{k_2}, \ldots\rangle\langle n_{k_1}, n_{k_2}, \ldots|, \tag{30} $$

which applies both in the presence and absence of interactions. Often we consider a system with a fixed number of indistinguishable particles. In that case, we can discard all terms in the completeness relation with the wrong number of particles and only keep terms for which $\sum_j n_{k_j} = N$.

Of course, all n_{k_j} are non-negative integers for bosons, while $n_{k_j} \in \{0, 1\}$ for fermions. In the following, we will use the convention that if one or more of the n_{k_j} in a Fock state take an invalid value, the Fock state should be replaced by zero.

1.4 Distinguishable and indistinguishable particles

What do we do, if the considered system consists of both distinguishable and indistinguishable particles, for instance one proton and two spin-polarized electrons? In that case, we group the particles, such that indistinguishable particles of the same type belong to the same group. In the example, the two spin-polarized electrons would form one group, and the proton would form another group. Let $|\psi_{i_j}\rangle$ be the i_jth basis ket of group j. If group j contains one particle, $|\psi_{i_j}\rangle$ is a single-particle state ket, and if it contains more than one particle, $|\psi_{i_j}\rangle$ is a Fock state ket. The quantum state of the system is then written as

$$|\psi\rangle = \sum_{i_1, i_2 \ldots, i_K} c_{i_1, i_2, \ldots, i_K} |\psi_{i_1}\rangle \otimes |\psi_{i_2}\rangle \otimes \ldots |\psi_{i_K}\rangle, \tag{31}$$

where K is the number of groups, and $c_{i_1, i_2, \ldots, i_K}$ are expansion coefficients determining the state.

2 Operators for bosons

So far we have discussed how to represent quantum states of many-particles. We will next consider operators. Our strategy will be to first introduce creation and annihilation operators that act in a simple way on Fock states, and then we will show how to write other operators in terms of the creation and annihilation operators. In this section, we will introduce creation and annihilation operators for bosons.

2.1 Creation and annihilation operators for bosons

We define the bosonic creation operator $a^\dagger_{k_j}$ as the linear operator that acts in the following way on Fock states

$$\begin{aligned} &a^\dagger_{k_j} |n_{k_1}, n_{k_2}, \ldots, n_{k_{j-1}}, n_{k_j}, n_{k_{j+1}} \ldots\rangle_+ \\ &\qquad = \sqrt{n_{k_j} + 1} |n_{k_1}, n_{k_2}, \ldots, n_{k_{j-1}}, n_{k_j} + 1, n_{k_{j+1}} \ldots\rangle_+. \end{aligned} \tag{32}$$

We can, of course, define operators as we like, but we will see below why this definition is useful. Note that (32) determines all matrix elements of $a^\dagger_{k_j}$. From (32), it also follows that

$$\begin{aligned} &a^\dagger_{k_j} |n_{k_1}, n_{k_2}, \ldots, n_{k_{j-1}}, n_{k_j} - 1, n_{k_{j+1}} \ldots\rangle_+ \\ &\qquad = \sqrt{n_{k_j}} |n_{k_1}, n_{k_2}, \ldots, n_{k_{j-1}}, n_{k_j}, n_{k_{j+1}} \ldots\rangle_+. \end{aligned} \tag{33}$$

The adjoint of this equation is

$$
\begin{aligned}
&{}_+\langle n_{k_1}, n_{k_2}, \ldots, n_{k_{j-1}}, n_{k_j} - 1, n_{k_{j+1}} \ldots | a_{k_j} \\
&\qquad = {}_+\langle n_{k_1}, n_{k_2}, \ldots, n_{k_{j-1}}, n_{k_j}, n_{k_{j+1}} \ldots | \sqrt{n_{k_j}}, \quad (34)
\end{aligned}
$$

where $a_{k_j} \equiv (a_{k_j}^\dagger)^\dagger$, and therefore

$$
\begin{aligned}
&{}_+\langle n_{k_1}, n_{k_2}, \ldots, n_{k_{j-1}}, n_{k_j} - 1, n_{k_{j+1}} \ldots | a_{k_j} | n_{k_1}, n_{k_2}, \ldots, n_{k_{j-1}}, n_{k_j}, n_{k_{j+1}} \ldots \rangle_+ \\
&\qquad = \sqrt{n_{k_j}}, \quad (35)
\end{aligned}
$$

while all other matrix elements of a_{k_j} are zero. From this, it follows that

$$
\begin{aligned}
&a_{k_j} | n_{k_1}, n_{k_2}, \ldots, n_{k_{j-1}}, n_{k_j}, n_{k_{j+1}} \ldots \rangle_+ \\
&\qquad = \sqrt{n_{k_j}} | n_{k_1}, n_{k_2}, \ldots, n_{k_{j-1}}, n_{k_j} - 1, n_{k_{j+1}} \ldots \rangle_+. \quad (36)
\end{aligned}
$$

The action of a_{k_j} is thus to annihilate a boson in the single-particle state $|k_j\rangle$, and we therefore denote a_{k_j} the annihilation operator.

Finally, we observe that

$$
\begin{aligned}
&a_{k_j}^\dagger a_{k_j} | n_{k_1}, n_{k_2}, \ldots, n_{k_{j-1}}, n_{k_j}, n_{k_{j+1}} \ldots \rangle_+ \\
&\qquad = a_{k_j}^\dagger \sqrt{n_{k_j}} | n_{k_1}, n_{k_2}, \ldots, n_{k_{j-1}}, n_{k_j} - 1, n_{k_{j+1}} \ldots \rangle_+ \\
&\qquad = n_{k_j} | n_{k_1}, n_{k_2}, \ldots, n_{k_{j-1}}, n_{k_j}, n_{k_{j+1}} \ldots \rangle_+. \quad (37)
\end{aligned}
$$

does + means bosons

The operator $n_{k_j} = a_{k_j}^\dagger a_{k_j}$ is thus a number operator that counts the number of bosons in the single-particle state $|k_j\rangle$. In this note, we use the same notation for the operator n_{k_j} and the number n_{k_j}, as they can be distinguished based on the context.

2.2 Commutation relations for bosons

Let us assume that $i < j$. Comparing

$$
\begin{aligned}
&a_{k_i}^\dagger a_{k_j}^\dagger | n_{k_1}, n_{k_2}, \ldots, n_{k_i}, \ldots, n_{k_j}, \ldots \rangle_+ \\
&\qquad = \sqrt{n_{k_i} + 1} \sqrt{n_{k_j} + 1} | n_{k_1}, n_{k_2}, \ldots, n_{k_i} + 1, \ldots, n_{k_j} + 1, \ldots \rangle_+ \quad (38)
\end{aligned}
$$

to

$$
\begin{aligned}
&a_{k_j}^\dagger a_{k_i}^\dagger | n_{k_1}, n_{k_2}, \ldots, n_{k_i}, \ldots, n_{k_j}, \ldots \rangle_+ \\
&\qquad = \sqrt{n_{k_j} + 1} \sqrt{n_{k_i} + 1} | n_{k_1}, n_{k_2}, \ldots, n_{k_i} + 1, \ldots, n_{k_j} + 1, \ldots \rangle_+, \quad (39)
\end{aligned}
$$

it follows that the annihilation operators commute, i.e.

$$
[a_{k_i}^\dagger, a_{k_j}^\dagger] = 0. \quad (40)
$$

This also holds for $i > j$ and $i = j$. Taking the adjoint gives

$$[a_{k_i}, a_{k_j}] = 0. \tag{41}$$

To obtain the commutator between $a^\dagger_{k_j}$ and a_{k_i}, we assume $i < j$ and compare

$$\begin{aligned} &a^\dagger_{k_j} a_{k_i} |n_{k_1}, n_{k_2}, \ldots, n_{k_i}, \ldots, n_{k_j}, \ldots\rangle_+ \\ &\qquad = \sqrt{n_{k_j} + 1}\sqrt{n_{k_i}} |n_{k_1}, n_{k_2}, \ldots, n_{k_i} - 1, \ldots, n_{k_j} + 1, \ldots\rangle_+ \end{aligned} \tag{42}$$

to

$$\begin{aligned} &a_{k_i} a^\dagger_{k_j} |n_{k_1}, n_{k_2}, \ldots, n_{k_i}, \ldots, n_{k_j}, \ldots\rangle_+ \\ &\qquad = \sqrt{n_{k_i}}\sqrt{n_{k_j} + 1} |n_{k_1}, n_{k_2}, \ldots, n_{k_i} - 1, \ldots, n_{k_j} + 1, \ldots\rangle_+. \end{aligned} \tag{43}$$

A similar derivation holds for $i > j$, so $a^\dagger_{k_j}$ and a_{k_i} commute for $i \neq j$. For $i = j$, we instead have

$$\begin{aligned} a_{k_i} a^\dagger_{k_i} |n_{k_1}, n_{k_2}, \ldots, n_{k_i}, \ldots\rangle_+ &= (n_{k_i} + 1) |n_{k_1}, n_{k_2}, \ldots, n_{k_i}, \ldots\rangle_+ \\ &= (a^\dagger_{k_i} a_{k_i} + 1) |n_{k_1}, n_{k_2}, \ldots, n_{k_i}, \ldots\rangle_+. \end{aligned} \tag{44}$$

Altogether, we thus have

$$[a_{k_i}, a^\dagger_{k_j}] = \delta_{ij}. \tag{45}$$

We thus see that the creation and annihilation operators are equivalent to the creation and annihilation operators for harmonic oscillators.

annihilation: a_{k_j} , creation: $a^\dagger_{k_j}$

3 Operators for fermions

In this section, we will introduce creation and annihilation operators for fermions.

3.1 Creation and annihilation operators for fermions

In the case of fermions, we define the creation operator $a^\dagger_{k_j}$ by the following action on Fock states

$$\begin{aligned} &a^\dagger_{k_j} |n_{k_1}, n_{k_2}, \ldots, n_{k_{j-1}}, n_{k_j}, n_{k_{j+1}} \ldots\rangle_- \\ &\qquad = (-1)^{N_j} \delta_{n_{k_j}, 0} |n_{k_1}, n_{k_2}, \ldots, n_{k_{j-1}}, n_{k_j} + 1, n_{k_{j+1}} \ldots\rangle_-, \end{aligned} \tag{46}$$

where

$$N_j \equiv \sum_{i=1}^{j-1} n_{k_i}. \tag{47}$$

For the time being, the factor $(-1)^{N_j}$ is simply part of our definition. We will see below why it is useful. Taking the adjoint gives

$$\begin{aligned} &{}_-\langle n_{k_1}, n_{k_2}, \ldots, n_{k_{j-1}}, n_{k_j}, n_{k_{j+1}} \ldots | a_{k_j} \\ &\qquad = {}_-\langle n_{k_1}, n_{k_2}, \ldots, n_{k_{j-1}}, n_{k_j} + 1, n_{k_{j+1}} \ldots | (-1)^{N_j} \delta_{n_{k_j}, 0}, \end{aligned} \tag{48}$$

and hence

$$-\langle n_{k_1}, n_{k_2}, \ldots, n_{k_{j-1}}, n_{k_j}, n_{k_{j+1}} \ldots | a_{k_j} | n_{k_1}, n_{k_2}, \ldots, n_{k_{j-1}}, n_{k_j}+1, n_{k_{j+1}} \ldots \rangle_- = (-1)^{N_j} \delta_{n_{k_j},0}, \quad (49)$$

while all other matrix elements of a_{k_j} are zero. From this we conclude that the action of the annihilation operator a_{k_j} is

$$a_{k_j} | n_{k_1}, n_{k_2}, \ldots, n_{k_{j-1}}, n_{k_j}, n_{k_{j+1}} \ldots \rangle_- = (-1)^{N_j} \delta_{n_{k_j},1} | n_{k_1}, n_{k_2}, \ldots, n_{k_{j-1}}, n_{k_j}-1, n_{k_{j+1}} \ldots \rangle_-. \quad (50)$$

The operator $a^\dagger_{k_j} a_{k_j}$ acts as

$$\begin{aligned} a^\dagger_{k_j} a_{k_j} | n_{k_1}, n_{k_2}, \ldots, n_{k_{j-1}}, n_{k_j}, n_{k_{j+1}} \ldots \rangle_- &= a^\dagger_{k_j} (-1)^{N_j} \delta_{n_{k_j},1} | n_{k_1}, n_{k_2}, \ldots, n_{k_{j-1}}, n_{k_j}-1, n_{k_{j+1}} \ldots \rangle_- \\ &= \delta_{n_{k_j},1} | n_{k_1}, n_{k_2}, \ldots, n_{k_{j-1}}, n_{k_j}, n_{k_{j+1}} \ldots \rangle_-, \end{aligned} \quad (51)$$

and since $n_{k_j} \in \{0, 1\}$, this means that $a^\dagger_{k_j} a_{k_j}$ is the number operator, which counts the number of fermions in the single-particle state $|k_j\rangle$.

3.2 Anti-commutation relations for fermions

Let us assume $i < j$ and compare

$$\begin{aligned} a^\dagger_{k_i} a^\dagger_{k_j} | n_{k_1}, n_{k_2}, \ldots, n_{k_i}, \ldots, n_{k_j}, \ldots \rangle_- &= a^\dagger_{k_i} (-1)^{\sum_{l=1}^{j-1} n_{k_l}} \delta_{n_{k_j},0} | n_{k_1}, n_{k_2}, \ldots, n_{k_i}, \ldots, n_{k_j}+1, \ldots \rangle_- \\ = (-1)^{\sum_{l=1}^{j-1} n_{k_l} + \sum_{l'=1}^{i-1} n_{k_{l'}}} \delta_{n_{k_i},0} \delta_{n_{k_j},0} | n_{k_1}, n_{k_2}, \ldots, n_{k_i}+1, \ldots, n_{k_j}+1, \ldots \rangle_- & \end{aligned} \quad (52)$$

to

$$\begin{aligned} a^\dagger_{k_j} a^\dagger_{k_i} | n_{k_1}, n_{k_2}, \ldots, n_{k_i}, \ldots, n_{k_j}, \ldots \rangle_- &= a^\dagger_{k_j} (-1)^{\sum_{l'=1}^{i-1} n_{k_{l'}}} \delta_{n_{k_i},0} | n_{k_1}, n_{k_2}, \ldots, n_{k_i}+1, \ldots, n_{k_j}, \ldots \rangle_- \\ = (-1)^{\sum_{l=1}^{j-1} n_{k_l} + 1 + \sum_{l'=1}^{i-1} n_{k_{l'}}} \delta_{n_{k_i},0} \delta_{n_{k_j},0} | n_{k_1}, n_{k_2}, \ldots, n_{k_i}+1, \ldots, n_{k_j}+1, \ldots \rangle_-. & \end{aligned} \quad (53)$$

The two expressions differ by a minus sign, and thus we conclude that $a^\dagger_{k_j}$ and $a^\dagger_{k_i}$ anti-commute, i.e.

$$a^\dagger_{k_i} a^\dagger_{k_j} + a^\dagger_{k_j} a^\dagger_{k_i} \equiv \{a^\dagger_{k_i}, a^\dagger_{k_j}\} = 0. \quad (54)$$

Taking the adjoint gives

$$\{a_{k_i}, a_{k_j}\} = 0. \tag{55}$$

Assuming $i > j$ leads to the same anti-commutation relation. It also holds for $i = j$ as $(a^\dagger_{k_i})^2 = 0$.

How about $a^\dagger_{k_j}$ and a_{k_i}? We will assume $i < j$ and compare

$$\begin{aligned} &a^\dagger_{k_j} a_{k_i} |n_{k_1}, n_{k_2}, \ldots, n_{k_i}, \ldots, n_{k_j}, \ldots\rangle_- \\ &= (-1)^{\sum_{l=1}^{j-1} n_{k_l} - 1 + \sum_{l'=1}^{i-1} n_{k_{l'}}} \delta_{n_{k_j},0} \delta_{n_{k_i},1} |n_{k_1}, n_{k_2}, \ldots, n_{k_i} - 1, \ldots, n_{k_j} + 1, \ldots\rangle_- \end{aligned} \tag{56}$$

to

$$\begin{aligned} &a_{k_i} a^\dagger_{k_j} |n_{k_1}, n_{k_2}, \ldots, n_{k_i}, \ldots, n_{k_j}, \ldots\rangle_- \\ &= (-1)^{\sum_{l=1}^{j-1} n_{k_l} + \sum_{l'=1}^{i-1} n_{k_{l'}}} \delta_{n_{k_j},0} \delta_{n_{k_i},1} |n_{k_1}, n_{k_2}, \ldots, n_{k_i} - 1, \ldots, n_{k_j} + 1, \ldots\rangle_-. \end{aligned} \tag{57}$$

Thus $a^\dagger_{k_j}$ and a_{k_i} anti-commute for $i < j$. The same applies for $i > j$. For $i = j$, we have

$$\begin{aligned} &a_{k_i} a^\dagger_{k_i} |n_{k_1}, n_{k_2}, \ldots, n_{k_i}, \ldots\rangle_- \\ &\qquad = a_{k_i} (-1)^{\sum_{l=1}^{i-1} n_{k_l}} \delta_{n_{k_i},0} |n_{k_1}, n_{k_2}, \ldots, n_{k_i} + 1, \ldots\rangle_- \\ &\qquad\qquad = \delta_{n_{k_i},0} |n_{k_1}, n_{k_2}, \ldots, n_{k_i}, \ldots\rangle_-. \end{aligned} \tag{58}$$

Combining this with (51), we see that

$$a_{k_i} a^\dagger_{k_i} + a^\dagger_{k_i} a_{k_i} = \delta_{n_{k_i},0} + \delta_{n_{k_i},1} = 1. \tag{59}$$

Altogether, we thus have the anti-commutation relation

$$\{a_{k_i}, a^\dagger_{k_j}\} = \delta_{ij} \tag{60}$$

for fermions.

4 Fock states from creation operators

With the above definitions of the bosonic and fermionic annihilation operators, we can write a general Fock state as

$$|n_{k_1} n_{k_2} n_{k_3} \ldots\rangle_\pm = (n_{k_1}! n_{k_2}! n_{k_3}! \cdots)^{-1/2} \left(a^\dagger_{k_1}\right)^{n_{k_1}} \left(a^\dagger_{k_2}\right)^{n_{k_2}} \left(a^\dagger_{k_3}\right)^{n_{k_3}} \ldots |0\rangle_\pm. \tag{61}$$

So one can get any Fock state by applying creation operators to the vacuum state. By creating the fermions furthest to the right first, we ensure that N_j

in the definition of the fermionic creation operator is always zero, and therefore no minus signs are accumulated. Note also that exchanging two fermions in the Fock state, means exchanging two of the creation operators, and this gives rise to a global minus sign.

We can also turn the above equation around and get a vacuum state by annihilating all the particles in the Fock state. Specifically

$$\dots (a_{k_3})^{n_{k_3}} (a_{k_2})^{n_{k_2}} (a_{k_1})^{n_{k_1}} |n_{k_1} n_{k_2} n_{k_3} \dots\rangle_\pm (n_{k_1}! n_{k_2}! n_{k_3}! \cdots)^{-1/2} = |0\rangle_\pm. \tag{62}$$

We can thus transform any Fock state into any Fock state by applying a product of creation and annihilation operators. Note also that if we apply the above sequence of annihilation operators to a different Fock state with the same total number of particles, we get zero because we annihilate particles that are not present in the state. We thus have operators that can pick out a particular basis state and transform it into a given basis state. By making linear combinations of these operators, we can express any linear operator in Fock space with a fixed number of particles in terms of creation and annihilation operators. Linear operators are what we need for quantum mechanics, so the theory can be expressed in terms of Fock states and creation and annihilation operators. This is one of the reasons why creation and annihilation operators are so central. Furthermore, annihilation and creation operators also allow us to model systems, in which the number of particles can change.

5 Basis transformations

A Hamiltonian often consists of different terms, and often some of these terms are simple in one basis, while other terms in the Hamiltonian are simple in another basis. An example is a kinetic energy term that is simple in the momentum basis and a potential energy term that is simple in the position basis. We therefore often need to do basis transformations.

Consider a complete set of single-particle states $|q\rangle$. We know how to write these states in terms of another complete set of single-particle states $|k\rangle$, namely through the basis transformation

$$|q\rangle = \sum_k \langle k|q\rangle |k\rangle. \tag{63}$$

If $b_q^\dagger$ is the operator that creates a particle in the state $|q\rangle$, and $a_k^\dagger$ is the operator that creates a particle in the state $|k\rangle$, we have

$$b_q^\dagger |0\rangle = \sum_k \langle k|q\rangle a_k^\dagger |0\rangle. \tag{64}$$

This suggests that

$$b_q^\dagger = \sum_k \langle k|q\rangle a_k^\dagger. \tag{65}$$

Indeed, for bosons

$$[b_q, b_{q'}^\dagger] = \sum_k \sum_{k'} \langle q|k\rangle\langle k'|q'\rangle [a_k, a_{k'}^\dagger] = \sum_k \sum_{k'} \langle q|k\rangle\langle k'|q'\rangle \delta_{kk'} = \langle q|q'\rangle = \delta_{qq'} \tag{66}$$

and $[b_q, b_{q'}] = 0$. For fermions, we just need to replace all [] by {}. This shows that (65) is a valid creation operator. Hence we can do the basis transformation directly on the creation and annihilation operators.

6 Operators in second quantization

In this section, we will give some examples of how one can write operators in terms of creation and annihilation operators. We start with the important observation that operators must be symmetric under exchange of indistinguishable particles. This is so because we want to stay within the same Fock space, but we only do so if an (anti-)symmetric state is transformed into an (anti-)symmetric state when we apply the operator.

6.1 One-particle operators

A one-particle operator is an operator that acts nontrivially only on a single particle at a time, i.e. it consists of terms like

$$1_1^{(1)} \otimes 1_1^{(2)} \otimes \cdots \otimes 1_1^{(i-1)} \otimes A_1^{(i)} \otimes 1_1^{(i+1)} \otimes \cdots \otimes 1_1^{(N)}. \tag{67}$$

Here, the subscript 1 indicates that the operator acts on a single particle, and the superscript says which particle the operator is acting on. A_1 is a general operator and 1_1 is the identity. Adding the requirement that operators must be symmetric under exchange of particles, we conclude that one-particle operators in systems with N particles must have the form

$$A_N = \sum_{i=1}^{N} 1_1^{(1)} \otimes 1_1^{(2)} \otimes \cdots \otimes 1_1^{(i-1)} \otimes A_1^{(i)} \otimes 1_1^{(i+1)} \otimes \cdots \otimes 1_1^{(N)}. \tag{68}$$

For simplicity of notation, this is often written as

$$A_N = \sum_{i=1}^{N} A_1^{(i)}. \tag{69}$$

We will here assume that $A_1^{(i)}$ is Hermitian, and we can hence find single-particle eigenstates for $A_1^{(i)}$, such that

$$A_1^{(i)}|k_i\rangle = \lambda_{k_i}|k_i\rangle, \tag{70}$$

where λ_{k_i} are the eigenvalues. Then

$$A_N|k_1k_2\dots k_N\rangle_\pm = \sum_{i=1}^{N} A_1^{(i)}|k_1k_2\dots k_N\rangle_\pm = \sum_{i=1}^{N}\lambda_{k_i}|k_1k_2\dots k_N\rangle_\pm \\ = \sum_k \lambda_k n_k |k_1k_2\dots k_N\rangle_\pm. \quad (71)$$

In the last line, we have put together the eigenvalues for particles in the same single-particle state, and the sum runs over all the allowed momenta of a single particle rather than over the N particles. As (71) applies for all (anti-)symmetrized product states, we conclude that

$$A_N = \sum_k \lambda_k n_k = \sum_k \lambda_k a_k^\dagger a_k = \sum_k \langle k|A_1|k\rangle a_k^\dagger a_k. \quad (72)$$

We can express this operator in a different basis as follows. First note that

$$\langle k|A_N|k'\rangle = \langle k|A_N|k\rangle\delta_{kk'} \quad (73)$$

because $|k\rangle$ is by definition the basis in which A_N is diagonal. This allows us to rewrite

$$A_N = \sum_k\sum_{k'}\langle k|A_1|k'\rangle a_k^\dagger a_{k'} = \sum_q\sum_{q'}\sum_k\sum_{k'}\langle k|q\rangle\langle q|A_1|q'\rangle\langle q'|k'\rangle a_k^\dagger a_{k'}. \quad (74)$$

In a general basis $|q\rangle$ with creation operator $b_q^\dagger$, we thus have

$$A_N = \sum_q\sum_{q'}\langle q|A_1|q'\rangle b_q^\dagger b_{q'}. \quad (75)$$

6.2 Two-particle operators

We will next consider a two-particle operator,

$$A_N = \frac{1}{2}\sum_{i\neq j} A_2^{(i,j)} \quad (76)$$

as they are also quite common. In this equation, $A_2^{(i,j)}$ acts on particles i and j, while the identity operator is applied to all other particles. We require $A_2^{(i,j)} = A_2^{(j,i)}$ because A_N must be symmetric under exchange of particles as discussed above. We divide by a factor of two because all particle pairs appear twice in the sum, and we require $i \neq j$, because the terms with $i = j$ are a one-particle operator.

In the following, we will assume that there exists a single-particle basis such that

$$A_2^{(i,j)}|k_i,k_j\rangle = \lambda_{k_i,k_j}|k_i,k_j\rangle \quad (77)$$

for all i and j simultaneously. If some particles are in the same single-particle state, some terms of the operator will be the same. In particular, if k and k' are different, and there are n_k particles in state $|k\rangle$ and $n_{k'}$ particles in state $|k'\rangle$, we have that $\lambda_{k,k'}$ appears $n_k n_{k'}$ times. Likewise, $\lambda_{k,k}$ appears $n_k(n_k-1)$ times in the sum. Thus

$$\begin{aligned} A_N|k_1\ldots,k_N\rangle &= \frac{1}{2}\sum_{i\neq j} A_2^{(i,j)}|k_1\ldots,k_N\rangle \\ &= \left[\frac{1}{2}\sum_{k\neq k'}\lambda_{k,k'}n_k n_{k'} + \frac{1}{2}\sum_k \lambda_{k,k}n_k(n_k-1)\right]|k_1\ldots,k_N\rangle \\ &= \frac{1}{2}\sum_k\sum_{k'}\lambda_{k,k'}\left[n_k n_{k'} - n_k\delta_{k,k'}\right]|k_1\ldots,k_N\rangle. \end{aligned} \quad (78)$$

We can rewrite

$$\begin{aligned} n_k n_{k'} - n_k\delta_{k,k'} = a_k^\dagger a_k a_{k'}^\dagger a_{k'} - a_k^\dagger a_k\delta_{k,k'} &= a_k^\dagger(\delta_{k,k'} \pm a_{k'}^\dagger a_k)a_{k'} - a_k^\dagger a_k\delta_{k,k'} \\ &= \pm a_k^\dagger a_{k'}^\dagger a_k a_{k'} = a_k^\dagger a_{k'}^\dagger a_{k'} a_k. \end{aligned} \quad (79)$$

We can hence write the second quantized form of the two-particle operator as

$$A_N = \frac{1}{2}\sum_k\sum_{k'}\langle kk'|A_2|kk'\rangle a_k^\dagger a_{k'}^\dagger a_{k'} a_k. \quad (80)$$

Again, one can do a basis transformation to obtain A_N in a general basis, which gives

$$A_N = \frac{1}{2}\sum_q\sum_{q'}\sum_{q''}\sum_{q'''}\langle q,q'|A_2|q'',q'''\rangle b_q^\dagger b_{q'}^\dagger b_{q'''} b_{q''}. \quad (81)$$

6.3 Example

As an example, we will write the Hamiltonian

$$H = \sum_i \frac{\mathbf{p}_i^2}{2m} + \frac{1}{2}\sum_{i\neq j} V(\mathbf{x}_j - \mathbf{x}_i) \quad (82)$$

in terms of annihilation and creation operators. Here, $\mathbf{x}_i$ is the position operator of particle i, $\mathbf{p}_i$ is the momentum operator of particle i, m is the mass of one of the indistinguishable particles, and V is a function that describes the interactions between the particles. The kinetic energy term is a single-particle operator, which is diagonal in the momentum basis. From (72), we thus have

$$\sum_i \frac{\mathbf{p}_i^2}{2m} = \sum_{\mathbf{k}}\langle\mathbf{k}|\frac{\mathbf{p}^2}{2m}|\mathbf{k}\rangle a_{\mathbf{k}}^\dagger a_{\mathbf{k}} = \sum_{\mathbf{k}}\frac{\hbar^2\mathbf{k}^2}{2m}a_{\mathbf{k}}^\dagger a_{\mathbf{k}}. \quad (83)$$

The second term of the Hamiltonian is an interaction that only depends on the relative coordinate of particles i and j. Equation (77) is thus fulfilled in the position basis. Here, however, we would like to express the operator in the momentum basis, as the first term of the Hamiltonian is simple in the momentum basis. From (81), the relevant matrix elements to compute are

$$\begin{aligned}
&\langle \mathbf{k}_1', \mathbf{k}_2' | V(\mathbf{x}_2 - \mathbf{x}_1) | \mathbf{k}_1, \mathbf{k}_2 \rangle \\
&\quad = \int d^3x_1 \int d^3x_2 \langle \mathbf{k}_1', \mathbf{k}_2' | \mathbf{x}_1, \mathbf{x}_2 \rangle \langle \mathbf{x}_1, \mathbf{x}_2 | V(\mathbf{x}_2 - \mathbf{x}_1) | \mathbf{k}_1, \mathbf{k}_2 \rangle \\
&\quad = \frac{1}{L^6} \int d^3x_1 \int d^3x_2 V(\mathbf{x}_2 - \mathbf{x}_1) e^{-i\mathbf{k}_1' \cdot \mathbf{x}_1 - i\mathbf{k}_2' \cdot \mathbf{x}_2 + i\mathbf{k}_1 \cdot \mathbf{x}_1 + i\mathbf{k}_2 \cdot \mathbf{x}_2}. \quad (84)
\end{aligned}$$

Introducing the center of mass and relative coordinates,

$$\mathbf{R} = \frac{1}{2}(\mathbf{x}_1 + \mathbf{x_2}), \qquad \mathbf{r} = \mathbf{x}_2 - \mathbf{x_1}, \tag{85}$$

we can rewrite this to

$$\begin{aligned}
&\langle \mathbf{k}_1', \mathbf{k}_2' | V(\mathbf{x}_2 - \mathbf{x}_1) | \mathbf{k}_1, \mathbf{k}_2 \rangle \\
&\quad = \frac{1}{L^6} \int d^3r \int d^3R\, V(\mathbf{r}) e^{i(\mathbf{k}_1 + \mathbf{k}_2 - \mathbf{k}_1' - \mathbf{k}_2') \cdot \mathbf{R}} e^{\frac{i}{2}((\mathbf{k}_1' - \mathbf{k}_2') - (\mathbf{k}_1 - \mathbf{k}_2)) \cdot \mathbf{r}} \\
&\quad = \delta_{\mathbf{k}_1 + \mathbf{k}_2, \mathbf{k}_1' + \mathbf{k}_2'} \frac{1}{L^3} \int d^3r\, V(\mathbf{r}) e^{\frac{i}{2}((\mathbf{k}_1' - \mathbf{k}_2') - (\mathbf{k}_1 - \mathbf{k}_2)) \cdot \mathbf{r}} \\
&\quad = \delta_{\mathbf{k}_1 + \mathbf{k}_2, \mathbf{k}_1' + \mathbf{k}_2'} \frac{1}{L^3} \int d^3r\, V(\mathbf{r}) e^{-i(\mathbf{k}_1 - \mathbf{k}_1') \cdot \mathbf{r}} \\
&\quad = \delta_{\mathbf{k}_1 + \mathbf{k}_2, \mathbf{k}_1' + \mathbf{k}_2'} \tilde{V}(\mathbf{k}_1 - \mathbf{k}_1'), \quad (86)
\end{aligned}$$

where

$$\tilde{V}(\mathbf{q}) \equiv \frac{1}{L^3} \int d^3r\, V(\mathbf{r}) e^{-i\mathbf{q} \cdot \mathbf{r}} \tag{87}$$

is the Fourier transform of $V(\mathbf{r})$. ← Function that describes interaction bt. particles.

We can thus write the interaction term in the Hamiltonian as

$$\frac{1}{2} \sum_{i \neq j} V(\mathbf{x}_j - \mathbf{x}_i) = \frac{1}{2} \sum_{\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_1', \mathbf{k}_2'} \delta_{\mathbf{k}_1 + \mathbf{k}_2, \mathbf{k}_1' + \mathbf{k}_2'} \tilde{V}(\mathbf{k}_1 - \mathbf{k}_1') a_{\mathbf{k}_1'}^\dagger a_{\mathbf{k}_2'}^\dagger a_{\mathbf{k}_2} a_{\mathbf{k}_1}. \tag{88}$$

Due to the delta function, we can reduce the four variables to three. We do this by defining

$$\mathbf{k}_1 \equiv \mathbf{k}, \quad \mathbf{k}_2 \equiv \mathbf{p}, \quad \mathbf{k}_1' \equiv \mathbf{k} - \mathbf{q}, \quad \mathbf{k}_2' = \mathbf{k}_1 + \mathbf{k}_2 - \mathbf{k}_1' = \mathbf{p} + \mathbf{q}. \tag{89}$$

This simplifies the expression for the interaction term to

$$\frac{1}{2} \sum_{i \neq j} V(\mathbf{x}_j - \mathbf{x}_i) = \frac{1}{2} \sum_{\mathbf{k}, \mathbf{p}, \mathbf{q}} \tilde{V}(\mathbf{q}) a_{\mathbf{k} - \mathbf{q}}^\dagger a_{\mathbf{p} + \mathbf{q}}^\dagger a_{\mathbf{p}} a_{\mathbf{k}}. \tag{90}$$

Note that the interaction conserves the total momentum $\mathbf{k}+\mathbf{p}$ of the two particles.

In conclusion, the Hamiltonian is

$$H = \sum_{\mathbf{k}} \frac{\hbar^2 \mathbf{k}^2}{2m} a^\dagger_{\mathbf{k}} a_{\mathbf{k}} + \frac{1}{2} \sum_{\mathbf{k},\mathbf{p},\mathbf{q}} \tilde{V}(\mathbf{q}) a^\dagger_{\mathbf{k}-\mathbf{q}} a^\dagger_{\mathbf{p}+\mathbf{q}} a_{\mathbf{p}} a_{\mathbf{k}}, \tag{91}$$

when written in terms of creation and annihilation operators.

A The cross product

The cross product

$$C = A \otimes B \tag{92}$$

of two matrices A and B is a matrix C with elements

$$C_{(i,k),(j,l)} = A_{i,j} B_{k,l}. \tag{93}$$

If A has dimensions $L_1 \times L_2$ and B has dimensions $M_1 \times M_2$, then C has dimensions $L_1 M_1 \times L_2 M_2$. As an example,

$$\begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix} \otimes \begin{pmatrix} B_{11} & B_{12} \end{pmatrix} = \begin{pmatrix} A_{11}B_{11} & A_{11}B_{12} & A_{12}B_{11} & A_{12}B_{12} \\ A_{21}B_{11} & A_{21}B_{12} & A_{22}B_{11} & A_{22}B_{12} \end{pmatrix}. \tag{94}$$

The following rules apply:

$$\langle a|b\rangle\langle c|d\rangle = (\langle a| \otimes \langle c|)(|b\rangle \otimes |d\rangle) \tag{95}$$

and

$$|a\rangle\langle b| \otimes |c\rangle\langle d| = (|a\rangle \otimes |c\rangle)(\langle b| \otimes \langle d|). \tag{96}$$

Both properties are derived by comparing the matrix elements on both sides of the equations. For example, if all the kets are represented by 2×1 matrices, then these equations say

$$\begin{aligned} \left[\begin{pmatrix} a_1^* & a_2^* \end{pmatrix} \begin{pmatrix} b_1 \\ b_2 \end{pmatrix}\right] \left[\begin{pmatrix} c_1^* & c_2^* \end{pmatrix} \begin{pmatrix} d_1 \\ d_2 \end{pmatrix}\right] &= (a_1^* b_1 + a_2^* b_2)(c_1^* d_1 + c_2^* d_2) \\ &= a_1^* b_1 c_1^* d_1 + a_1^* b_1 c_2^* d_2 + a_2^* b_2 c_1^* d_1 + a_2^* b_2 c_2^* d_2 \\ &= \begin{pmatrix} a_1^* c_1^* & a_1^* c_2^* & a_2^* c_1^* & a_2^* c_2^* \end{pmatrix} \begin{pmatrix} b_1 d_1 \\ b_1 d_2 \\ b_2 d_1 \\ b_2 d_2 \end{pmatrix} \\ &= \left[\begin{pmatrix} a_1^* & a_2^* \end{pmatrix} \otimes \begin{pmatrix} c_1^* & c_2^* \end{pmatrix}\right] \left[\begin{pmatrix} b_1 \\ b_2 \end{pmatrix} \otimes \begin{pmatrix} d_1 \\ d_2 \end{pmatrix}\right] \end{aligned} \tag{97}$$

and

$$\left[\begin{pmatrix} a_1 \\ a_2 \end{pmatrix} \begin{pmatrix} b_1^* & b_2^* \end{pmatrix}\right] \otimes \left[\begin{pmatrix} c_1 \\ c_2 \end{pmatrix} \begin{pmatrix} d_1^* & d_2^* \end{pmatrix}\right] =$$
$$\begin{pmatrix} a_1 b_1^* & a_1 b_2^* \\ a_2 b_1^* & a_2 b_2^* \end{pmatrix} \otimes \begin{pmatrix} c_1 d_1^* & c_1 d_2^* \\ c_2 d_1^* & c_2 d_2^* \end{pmatrix} =$$
$$\begin{pmatrix} a_1 c_1 \\ a_1 c_2 \\ a_2 c_1 \\ a_2 c_2 \end{pmatrix} \begin{pmatrix} b_1^* d_1^* & b_1^* d_2^* & b_2^* d_1^* & b_2^* d_2^* \end{pmatrix} =$$
$$\left[\begin{pmatrix} a_1 \\ a_2 \end{pmatrix} \otimes \begin{pmatrix} c_1 \\ c_2 \end{pmatrix}\right] \left[\begin{pmatrix} b_1^* & b_2^* \end{pmatrix} \otimes \begin{pmatrix} d_1^* & d_2^* \end{pmatrix}\right]. \quad (98)$$

References

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