Second Quantization

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Abstract

This note introduces key concepts in second quantization. How many-body states are symmetrized and then normalized to give Fock states is explained in detail. The matrix elements of 1- and 2-body operators under the Fock basis are calculated.

Prerequisites include projectors, subspaces, and basic notions about quantum states and Hilbert spaces. Ref. [1, §1.2] is the main reference for this note. Comments on other sources are given in the bibliographical notes section.

Contents

1 Physical subspaces and their projectors

Motivation 1.1. In 3 spatial dimensions, there are only two types of exchange statistics of quantum-mechanical particles. [1] These are Bosonic statistics where permutations are trivial, and Fermionic statistics where the wavefunction changes sign upon an odd permutation. This bears consequences for wavefunctions. For example, if two particles are identical, then the direct product state $|0\rangle \otimes |1\rangle$ becomes unphysical: it is neither Bosonic (which should be $|01\rangle + |10\rangle$) nor Fermionic (which should be $|01\rangle - |10\rangle$). We are therefore motivated to study how physical states can be constructed from arbitrary product states.

To specify the exchange statistics, we must label the particles, but in reality we can not do this for identical particles. Labelling is purely for the sake of narration. In fact, we will arrive at the so-called occupation number representation where labelling is impossible.

Before trying to construct physical states we first introduce some tools needed to define "physical".

Definition 1.1. A *permutation* is a function

$$P : \{(12 \cdots N)\} \mapsto \{(12 \cdots N)\}, (123 \cdots N) \mapsto (P1, P2, \dots, PN) \tag{1.1}$$

[1] In (2+1)D there exist particles that are neither Fermions nor Bosons, known as "anyons". We shall see in this note that Boson/Fermion statistics is closely tied to permutations (which form a group). Similarly, anyon statistics is closely tied to braids (which also form a group).

where $\{(12\cdots N)\}$ denotes all possible N-bit strings consisting of the integers 1,2, ..., N. P is defined to be *even* if it can be realized (*i.e.* implemented) by an even number of exchanges, and *odd* if it can be realized by an odd number of exchanges. [2] We define $|P| = 1$ for even permutations and $|P| = -1$ for odd ones; $|P|$ is known as the *signature* or *parity* of P.

For example, $P : (123) \mapsto (213)$ is odd, while $P' : (123) \mapsto (231)$ is even. For any permutation P, $|P| = \left|P^{-1}\right|$ where P^{-1} is the inverse of the permutation. [3]

Definition 1.2 (Bosonic and Fermionic projectors)**.** For an N-particle product state

$$|\alpha_1, \alpha_2, \ldots, \alpha_N) \coloneqq |\alpha_1\rangle \otimes |\alpha_2\rangle \cdots \otimes |\alpha_N\rangle \tag{1.2}$$

where $\forall i, |\alpha_i\rangle \in \{|\lambda_1\rangle, \ldots, |\lambda_d\rangle\}$ and $\{|\lambda_j\rangle\}_{j=1}^d$ is an orthonormal basis of the 1-body Hilbert space, the Bosonic (Fermionic) projector $\mathcal{P}_B$ ($\mathcal{P}_F$) are defined in terms of their action on product states,

$$\mathcal{P}_B|\alpha_1, \ldots, \alpha_N) \coloneqq \frac{1}{N!}\sum_P \zeta^{|P|}|\alpha_{P1}, \ldots, \alpha_{PN}) \quad \text{with } \zeta = 1, \tag{1.3}$$

$$\mathcal{P}_F|\alpha_1, \ldots, \alpha_N) \coloneqq \frac{1}{N!}\sum_P \zeta^{|P|}|\alpha_{P1}, \ldots, \alpha_{PN}) \quad \text{with } \zeta = -1. \tag{1.4}$$

When the distinction between Bosons and Fermions does not matter we use $\mathcal{P}$ to denote $\mathcal{P}_B$ or $\mathcal{P}_F$. The operators $\mathcal{P}_B, \mathcal{P}_F$ are obviously linear.

Now we can define what we mean by "physical" using these projectors.

Definition 1.3 (Bosonic and Fermionic states)**.** For any N-body state $|\Psi\rangle$, we can project it onto the product basis $\{|\alpha_1, \ldots, \alpha_N)\}$, obtaining $|\Psi\rangle = \sum_{\alpha_1,\ldots,\alpha_N} C_{\alpha_1,\ldots,\alpha_N}|\alpha_1, \ldots, \alpha_N)$, and then apply the projectors as previously defined. We define that $|\Psi\rangle$ is Bosonic if it is preserved by $\mathcal{P}_B$ and Fermionic if it is preserved by $\mathcal{P}_F$. It follows that all Bosonic states form a subspace $\mathcal{H}_B \coloneqq \{|\Psi\rangle : \mathcal{P}_B\,|\Psi\rangle = |\Psi\rangle\}$ and all Fermionic states form a subspace $\mathcal{H}_F \coloneqq \{|\Psi\rangle : \mathcal{P}_F\,|\Psi\rangle = |\Psi\rangle\}$ of the total product Hilbert space.

We have called $\mathcal{P}_B, \mathcal{P}_F$ projectors but are they? Let us check idempotence explicitly.

$$\begin{aligned}
\mathcal{P}^2|\alpha_1, \ldots, \alpha_N) &= \frac{1}{N!}\sum_{P'}\zeta^{|P'|}\frac{1}{N!}\sum_P \zeta^{|P|}|\alpha_{P'P1}, \ldots, \alpha_{P'PN}) \\
&= \frac{1}{N!}\sum_{P'}\frac{1}{N!}\sum_P \zeta^{|P'P|}|\alpha_{P'P1}, \ldots, \alpha_{P'PN}) \\
&= \frac{1}{N!}\sum_{P'}\frac{1}{N!}\sum_{P'P} \zeta^{|P'P|}|\alpha_{P'P1}, \ldots, \alpha_{P'PN}) \\
&= \mathcal{P}|\alpha_1, \ldots, \alpha_N),
\end{aligned}$$

where in the second-to-last line the operator $\frac{1}{N!}\sum_{P'}$ equals to identity because it only involves superposition, not permutation. [4]

The idenpotence of $\mathcal{P}$ means $\mathcal{P}(\mathcal{P}\,|\psi\rangle) = \mathcal{P}\,|\psi\rangle$, *i.e.* for any $|\psi\rangle$ the projected state $\mathcal{P}\,|\psi\rangle$ belongs to the subspace $\{|\Psi\rangle : \mathcal{P}\,|\Psi\rangle = |\Psi\rangle\}$.

Result 1.1. Given any many-body product state $|\alpha_1, \alpha_2, \ldots, \alpha_N)$, $\mathcal{P}_B|\alpha_1, \alpha_2, \ldots, \alpha_N) \in \mathcal{H}_B$, and similarly $\mathcal{P}_F|\alpha_1, \alpha_2, \ldots, \alpha_N) \in \mathcal{H}_F$. Physically, this means physical states are constructed via "scrambling" product states with the operator $\mathcal{P}$. This is known as the symmetrization of states.

[2] Formally proving that given a permutation this realization is either even or odd, and that this property does not depend on the specific way of realizing the permutation, is not within the scope of this note.

[3] Again, we don't formally prove this. Intuitively this is natural. Any permutation can be implemented via some steps of exchanges, and we can always invert a permutation by doing all its steps in reverse, and obviously this gives the same parity as the permutation itself.

[4] If the relabelling of summation variables from P', P to $P'P, P'$ seems strange, we can convince ourselves by noting that there exists a bijective mapping between $\{(P', P)\}$ and $\{(P'P, P)\}$.

Remark 1.1. Consistency requires that no state can be simultaneously Bosonic and Fermionic. Formally this manifests in the fact that $\mathcal{P}_B$ maps all Fermionic states to the null vector and hence $\mathcal{H}_B \perp \mathcal{H}_F$. Let us check this explicitly: for a Fermionic state $\mathcal{P}_F|\alpha_1, \ldots, \alpha_N)$,

$$\begin{aligned}
\frac{1}{N!}\sum_{P'}(+1)^{|P'|}\frac{1}{N!}\sum_{P}(-1)^{|P|}|\alpha_{P'P1}, \ldots, \alpha_{P'PN}) &= \frac{1}{N!}\sum_{P'}(-1)^{|P'|}\frac{1}{N!}\sum_{P'P}(-1)^{|P'P|}|\alpha_{P'P1}, \ldots, \alpha_{P'PN}) \\
&= \frac{1}{N!}\left(\sum_{\text{odd } P'} + \sum_{\text{even } P'}\right)(-1)^{|P'|}\mathcal{P}_F|\alpha_1, \ldots, \alpha_N) \\
&= 0,
\end{aligned}$$

where the first equality holds because whatever the parity of P', $(-1)^{2|P'|}$ is always 1, and the third equality holds because for each even P' there is an odd one that cancels its contribution.

2 The orthonormal Fock basis

Motivation 2.1. We would like to construct orthonormal bases within $\mathcal{H}_B$ and $\mathcal{H}_F$. Having taken care of exchange statistics, we now normalize the symmetrized state. After that we shall study whether the normalized states are orthogonal.

We calculate $\|\mathcal{P}|\alpha_1, \ldots, \alpha_N)\|$ by taking the inner product $(\alpha_1, \ldots, \alpha_N|\mathcal{P}^\dagger\mathcal{P}|\alpha_1, \ldots, \alpha_N)$ and taking its square root. Here it would be ideal if $\mathcal{P}$ was Hermitian, because in that case we can use idempotence and reduce the inner product to

$$(\alpha_1, \ldots, \alpha_N|\mathcal{P}|\alpha_1, \ldots, \alpha_N),$$

which is easy to calculate thanks to the orthogonality of the product basis.

We establish Hermiticity by verifying that $\mathcal{P}$ meets the Hermiticity condition: for any product states $|\alpha_1, \ldots, \alpha_N)$ and $|\alpha'_1, \ldots, \alpha'_N)$,

$$(\alpha_1, \ldots, \alpha_N|\mathcal{P}|\alpha'_1, \ldots, \alpha'_N) = (\alpha'_1, \ldots, \alpha'_N|\mathcal{P}|\alpha_1, \ldots, \alpha_N)^*, \tag{2.1}$$

which is equivalent to

$$\sum_P \zeta^{|P|}(\alpha_1, \ldots, \alpha_N|\alpha'_{P1}, \ldots, \alpha'_{PN}) = \sum_{P'} \zeta^{|P'|}(\alpha_{P'1}, \ldots, \alpha_{P'N}|\alpha'_1, \ldots, \alpha'_N).$$

Each LHS term

$$\zeta^{|P|}(\alpha_1, \ldots, \alpha_N|\alpha'_{P1}, \ldots, \alpha'_{PN})$$

can be equated (via applying P^{-1} on the "bra" and the "ket" simultaneously) with the RHS term

$$\zeta^{|P^{-1}|}(\alpha_{P^{-1}1}, \ldots, \alpha_{P^{-1}N}|\alpha'_1, \ldots, \alpha'_N),$$

where $\zeta^{|P|} = \zeta^{|P^{-1}|}$ and the inner product between two product states is always preserved by a simultaneous permutation, which proves eqn. (2.1).

Continuing with our task of normalization,

$$\begin{aligned}
&\|\mathcal{P}|\alpha_1, \ldots, \alpha_N)\|^2 \\
&= (\alpha_1, \ldots, \alpha_N|\sum_P \zeta^{|P|}\frac{1}{N!}|\alpha_{P1}, \ldots, \alpha_{PN}) \\
&= \frac{1}{N!}\prod_{n_{\lambda_i}\neq 0} n_{\lambda_i}! \quad \text{for Bosons, and } \frac{1}{N!} \quad \text{for Fermions,}
\end{aligned}$$

where in the last equality, contributing permutations are determined by the orthogonality of the product basis, and in particular the only contributing permutation in the Fermion case is the identity. The condition $n_{\lambda_i} \neq 0$ in the product is imposed so that the product does not vanish.

Result 2.1. After normalization the vector $\mathcal{P}|\alpha_1, \ldots, \alpha_N)$ becomes

$$\frac{\sqrt{N!}}{\sqrt{\prod_{n_{\lambda_i} \neq 0} n_{\lambda_i}!}} \mathcal{P}|\alpha_1, \ldots, \alpha_N).$$

Motivated by this result we define:

Definition 2.1. The normalized and symmetrized state

$$|\alpha_1, \ldots, \alpha_N\rangle \coloneqq \frac{\sqrt{N!}}{\sqrt{\prod_{n_{\lambda_i} \neq 0} n_{\lambda_i}!}} \mathcal{P}|\alpha_1, \ldots, \alpha_N) = \frac{\sqrt{N!}}{\sqrt{\prod_{n_{\lambda_i} \neq 0} n_{\lambda_i}!}} \frac{1}{N!} \sum_P \zeta^{|P|} |\alpha_1, \ldots, \alpha_N) \tag{2.2}$$

and the "partially normalized" state [5]

$$|\alpha_1, \ldots, \alpha_N\} \coloneqq \sqrt{N!} \mathcal{P}|\alpha_1, \ldots, \alpha_N). \tag{2.3}$$

Note that the partially normalized state and the normalized state are only different in the Bosonic case, because they only differ in the prefactor $(\prod n_{\lambda_i}!)^{1/2}$.

Having obtained normalized states, we go on to study their orthogonality. For this purpose we note that the only information carried by $|\alpha_1, \ldots, \alpha_N\rangle$ is

1. Which 1-body states among $\{|\lambda_i\rangle\}_{i=1}^d$ are occupied, and
2. for each occupied 1-body state, how many particles occupy it.

We can therefore encode these information in the following notation,

Definition 2.2 (Occupation number representation)**.** For the N-body normalized state $|\alpha_1, \ldots, \alpha_N\rangle$, the *occupation number representation* (also known as the Fock state) is $|n_{\lambda_1}, \ldots, n_{\lambda_d}\rangle$ where n_{λ_j} is the number of particles in the state $|\lambda_j\rangle$ and $\sum_{j=1}^d n_{\lambda_j} = N$.

Immediately we see that the Fock state carries the two pieces of information we mentioned. The unoccupied 1-body states have occupation number zero. Besides, it is impossible to label particles in the occupation number representation.

With this compact notation we study orthogonality. Intuitively we would expect $n_{\lambda_1} \neq n'_{\lambda_1}$ to imply

$$\langle n_{\lambda_1}, \ldots | n'_{\lambda_1}, \ldots \rangle = 0, \tag{2.4}$$

since the occupation number of $|\lambda_1\rangle$ *completely distinguishes between* these states and consequently their overlap should vanish. [6]

Now let us verify orthogonality explicitly. Denote $\sum_{\lambda_i} n_{\lambda_i}$ with N, and $\sum_{\lambda_i} n'_{\lambda_i}$ with M.

If $N = M$, we illustrate with an example; generalization is trivial. Say $n_{\lambda_1} = 2$ and $n'_{\lambda_1} = 1$. In the inner product $\langle n_{\lambda_1}, \ldots | n'_{\lambda_1}, \ldots \rangle$, each side is decomposed into a sum over product states. Whatever the permutation, $|\lambda_1\rangle$ always appear twice in the LHS and once in the RHS, so there is at least one $\langle \lambda_1|$ in the LHS which is taken inner product with a 1-body state that is not $|\lambda_1\rangle$, hence the inner product vanishes. This analysis extends to every term in the sum, so the total inner product vanishes.

If $N \neq M$ (say $N < M$), then we have to first consider what exactly we mean by the inner product between an N-body product state and an M-body product state. By the definition of inner product, we have to write the N-body product state as an M-body product state, and the only sensible way to do this

[5] The "partially normalized" state is useful in some miscellaneous situations, but it is not our primary focus, since we have not finished the task of finding an orthonormal basis.

[6] More concretely, if there exists a Hermitian operator $\hat{n}_{\lambda_1}$ which extracts the occupation number of $|\lambda_1\rangle$, then these two states belong to different eigenspaces of $\hat{n}_{\lambda_1}$, so they must be orthogonal. We will see in remark 2.1 that there indeed exists such an operator.

is to tensor it with $(M-N)$ 1-body null vectors, since this is the only way to guarantee nothing happens in the $(M-N)$ 1-body Hilbert spaces. Given this assumption, eqn. (2.4) follows. [7]

Result 2.2. Normalizing the symmetrized states and switching to the occupation number representation gives an orthonormal basis in the physical Hilbert spaces, known as the Fock basis. A Fock state is $|n_{\lambda_1}, \ldots, n_{\lambda_d}\rangle$ where n_{λ_j} is the number of particles in the state $|\lambda_j\rangle$ and $\sum_{j=1}^{d} n_{\lambda_j} = N$.

Remark 2.1. Because the Fock states are orthonormal, we can (but might choose not to) *define* the number operator in terms of how it acts on Fock states:

$$\hat{n}_{\lambda_i} |\cdots, n_{\lambda_i}, \ldots\rangle = n_{\lambda_i} |\cdots, n_{\lambda_i}, \ldots\rangle .$$

It follows that

$$\langle \cdots, n_{\lambda_i}, \ldots| \hat{n}_{\lambda_i}^{\dagger} = n_{\lambda_i}^{*} \langle \cdots, n_{\lambda_i}, \ldots| = n_{\lambda_i} \langle \cdots, n_{\lambda_i}, \ldots|$$

and the Hermitian condition

$$\langle \cdots, n_{\lambda_i}, \ldots| \hat{n}_{\lambda_i} |\cdots, n'_{\lambda_i}, \ldots\rangle = \langle \cdots, n'_{\lambda_i}, \ldots| \hat{n}_{\lambda_i} |\cdots, n_{\lambda_i}, \ldots\rangle^{*}$$

is met because, thanks to the orthogonality of the Fock basis, both sides in this equation are $n_{\lambda_i}\delta_{n_{\lambda_i}, n'_{\lambda_i}}$.

Remark 2.2. In the preceding discussion, all Fock states with total particle number $N \geq 1$ can be constructed via symmetrizing and normalizing product states. However, the Fock state $|0\rangle$ with total particle number zero seems difficult to make sense of, since we can not project it onto product states. We will gradually see the physical picture of this state in the next section.

Remark 2.3. Different Fock states can correspond to the same set of occupation numbers. For example, consider two Fermionic states with 1-body space $\{|\alpha\rangle, |\beta\rangle\}$: $|\alpha\beta\rangle \propto |\alpha\beta) - |\beta\alpha)$ and $|\beta\alpha\rangle \propto |\beta\alpha) - |\alpha\beta)$. They correspond to the same occupation numbers $n_\alpha = 1, n_\beta = 1$, but differ by an overall phase -1. In practice we always choose a ordering convention of writing down 1-body states so that this overall phase does not mess up our calculations. For example, to get rid of the -1 phase mentioned above, we can choose to always write $|\alpha\rangle$ before $|\beta\rangle$ in a Fock state. More generally, we might choose to always write down low-energy 1-body states before high-energy ones.

3 Creation and annihilation

Motivation 3.1. Previously we were motivated by the need to take care of exchange statistics of quantum states. But there is more to second quantization. Under the Fock basis, quantum states are labelled by their occupation numbers, *i.e.* the occupation numbers become degrees of freedom. We are thus motivated to study processes that manipulate these degrees of freedom. We will construct operators that do this and study their properties.

3.1 Creation, annihilation and number operators

Definition 3.1 (Creation operator)**.** The *creation operator* $\hat{\psi}_\alpha$ "creates" one particle in the 1-body state $|\alpha\rangle$. To be specific, it is defined by its action on a partially normalized state,

$$\hat{\psi}_\alpha |\alpha_1, \ldots, \alpha_N\} = |\alpha\alpha_1, \ldots, \alpha_N\} \tag{3.1}$$

with $\alpha, \alpha_1, \ldots, \alpha_N$ not necessarily different. Note that α is written on the left of the state $|\alpha\alpha_1, \ldots, \alpha_N\}$; recalling remark 2.3, this convention should be obeyed consistently to avoid confusion.

[7] We will see that the orthogonality of states with different total particle numbers is also required by the definition of creation and annihilation operators. However, in arguing in terms of product states here, we get a more intuitive understanding.

Fock states are related to partially normalized states as

$$|\alpha\alpha_1,\ldots,\alpha_N\} = \sqrt{\prod_{\alpha_i\neq\alpha} n_{\alpha_i}!}\sqrt{(n_\alpha+1)!}\,|\alpha\alpha_1,\ldots,\alpha_N\rangle\,,$$

$$|\alpha_1,\ldots,\alpha_N\} = \sqrt{\prod_{\alpha_i} n_{\alpha_i}!}\,|\alpha_1,\ldots,\alpha_N\rangle\,,$$

hence the creation operator acts on Fock states as

$$\begin{aligned}\hat{\psi}^\dagger_\alpha\,|\alpha_1,\ldots,\alpha_N\rangle &= \hat{\psi}^\dagger_\alpha\frac{1}{\sqrt{\prod_{\alpha_i} n_{\alpha_i}}}|\alpha_1,\ldots,\alpha_N\} \\ &= \frac{1}{\sqrt{\prod_{\alpha_i} n_{\alpha_i}}}|\alpha\alpha_1,\cdots,\alpha_N\} \\ &= \sqrt{n_\alpha+1}\,|\alpha\alpha_1,\ldots,\alpha_N\rangle\,.\end{aligned}$$

Motivation 3.2. $\hat{\psi}^\dagger_\alpha$ maps an N-body state to an $(N+1)$-body state, *i.e.* it looks like

$$\sum_N |(N+1)\text{-body state}\rangle\,\langle N\text{-body state}|\,.$$

We therefore expect $\hat{\psi}_\alpha$, its Hermitian adjoint, to map an $(N+1)$-body state to an N-body state, which can be interpreted as the "annihilation" of a particle. Let us study the properties of $\hat{\psi}_\alpha$ to check our intuition.

We project $\hat{\psi}_\alpha|\alpha'_1,\ldots,\alpha'_m\}$ onto $\{\alpha_1,\ldots,\alpha_n|$ to study a matrix element of $\hat{\psi}_\alpha$.

$$\begin{aligned}\{\alpha_1,\ldots,\alpha_n|\hat{\psi}_\alpha|\alpha'_1,\ldots,\alpha'_m\} &= \{\alpha'_1,\ldots,\alpha'_m|\hat{\psi}^\dagger_\alpha|\alpha_1,\ldots,\alpha_n\}^* \\ &= \{\alpha'_1,\ldots,\alpha'_m|\alpha\alpha_1,\ldots,\alpha_n\}^*.\end{aligned}$$

Therefore the only nonvanishing matrix elements are those where $m = n+1$.

Now we project $\hat{\psi}_\alpha|\alpha'_1,\ldots,\alpha'_m\}$ onto a complete basis $\{|\alpha_1,\ldots,\alpha_n\}\}$ where $n = m-1$ to obtain the formula of $\hat{\psi}_\alpha|\alpha'_1,\ldots,\alpha'_m\}$. For this purpose we need the identity within the n-body space

$$\mathbb{1}_n = \sum_{\alpha_1,\ldots,\alpha_n} |\alpha_1,\ldots,\alpha_n)(\alpha_1,\ldots,\alpha_n|,$$

which becomes

$$\mathbb{1}_n = \sum_{\alpha_1,\ldots,\alpha_n}\frac{1}{n!}|\alpha_1,\ldots,\alpha_n\}\{\alpha_1,\ldots,\alpha_n|$$

when expressed in terms of the basis $\{|\alpha_1,\ldots,\alpha_n\}\}$.

Proceeding with our expansion,

$$\begin{aligned}\hat{\psi}_\alpha|\alpha'_1,\ldots,\alpha'_m\} &= \sum_{\alpha_1,\ldots,\alpha_n}\frac{1}{n!}\{\alpha_1,\ldots,\alpha_n|\hat{\psi}_\alpha|\alpha'_1,\ldots,\alpha'_m\}\times|\alpha_1,\ldots,\alpha_n\} \\ &= \sum_{\alpha_1,\ldots,\alpha_{m-1}}\frac{1}{(m-1)!}\sqrt{m!}(\alpha\alpha_1,\ldots,\alpha_n|\frac{1}{m!}\sum_P\zeta^{|P|}|\alpha'_{P1},\ldots,\alpha'_{Pm})\sqrt{m!}\times|\alpha_1,\ldots,\alpha_{m-1}\}\end{aligned}$$

where the permutation P involves m indices, while the vector $|\alpha_1,\ldots,\alpha_{m-1}\}$ involves $m-1$ indices. The orthogonality of the product basis gives

$$\hat{\psi}_\alpha|\alpha'_1,\ldots,\alpha'_m\} = \frac{1}{(m-1)!}\sum_P\zeta^{|P|}\delta_{\alpha,\alpha'_{P1}}|\alpha'_{P2},\ldots,\alpha'_{Pm}\}.$$

But we want to express our result in a way not involving permuted indices, so we carry out the following permutation [8] for the state $|\alpha'_{P2},\dots,\alpha_{Pm}\}$:

$$(P1,P2,\dots,Pm)\mapsto(P1,1,2,3,\dots,P1-1,P1+1,\dots,m),$$

which is P^{-1} followed by $(P1-1)$ nearest-neighbor transpositions and has therefore the signature $\left|P^{-1}\right|+P1-1$. After this permutation, the ζ prefactor becomes $\zeta^{|P|+\left|P^{-1}\right|+P1-1}=\zeta^{P1-1}$, resulting in

$$\begin{aligned}
\hat{\psi}_\alpha|\alpha'_1,\dots,\alpha'_m\} &= \frac{1}{(m-1)!}\sum_P \zeta^{P1-1}\delta_{\alpha,\alpha'_{P1}}|\alpha'_1,\dots,\alpha'_{P1-1},\alpha'_{P1+1},\dots,\alpha'_{Pm}\} \\
&= \left(\sum_{P1=1}+\sum_{P1=2}+\cdots+\sum_{P1=m}\right)\frac{1}{(m-1)!}\zeta^{P1-1}\delta_{\alpha,\alpha'_{P1}}|\alpha'_1,\dots,\alpha'_{P1-1},\alpha'_{P1+1},\dots,\alpha'_{Pm}\} \\
&= \sum_{j=1}^{m}\zeta^{j-1}\delta_{\alpha,\alpha'_j}\left|\alpha'_1,\dots,\alpha'_{j-1},\alpha'_{j+1},\dots,\alpha'_m\right\},
\end{aligned}$$

where the last equation holds because the summand in the second-to-last line only depends on $P1$, so for each summation in the bracket $(\sum_{P1=1}+\sum_{P1=2}+\cdots+\sum_{P1=m})$, there are $(m-1)!$ identical terms, which cancels the prefactor $1/(m-1)!$.

This equation says to: 1) go to the index j in the array $(\alpha'_1,\dots,\alpha'_m)$ and check whether $\alpha'_j=\alpha$, 2) if yes, register a contributing term $\zeta^{j-1}|\alpha'_1,\dots,\alpha'_{j-1},\alpha'_{j+1},\dots,\alpha'_m\}$, 3) if no, don't register any contribution, and 4) sum up the contributing terms. Therefore, the sum $\sum_{j=1}^m$ picks up n_α contributing terms, all of which having one less particle in the 1-body state $|\alpha\rangle$ than the state $|\alpha'_1,\dots,\alpha'_m\}$.

In terms of Fock states,

$$\hat{\psi}_\alpha\left|\alpha'_1,\dots,\alpha'_m\right\rangle\times\sqrt{\prod_{\alpha'\neq\alpha}n_{\alpha'}}\sqrt{n_\alpha!}=\sum_{j=1}^{m}\zeta^{j-1}\delta_{\alpha,\alpha'_j}\left|\alpha'_1,\dots,\alpha'_{j-1},\alpha'_{j+1},\cdots,\alpha'_m\right\rangle\times\sqrt{\prod_{\alpha'\neq\alpha}n_{\alpha'}}\sqrt{(n_\alpha-1)!},$$

hence

$$\hat{\psi}_\alpha\left|\alpha'_1,\dots,\alpha'_m\right\rangle=\begin{cases}|\text{null}\rangle & \text{if } n_\alpha=0,\\ n_\alpha^{-1/2}\sum_{j=1}^m\zeta^{j-1}\delta_{\alpha,\alpha'_j}\left|\alpha'_1,\dots,\alpha'_{j-1},\alpha'_{j+1},\cdots,\alpha'_m\right\rangle & \text{if } n_\alpha\neq 0,\end{cases}$$

where for the case $n_\alpha=1$, the factor $\sqrt{(n_\alpha-1)!}$ is not multiplied, because such factors are only considered when the occupation number is not zero, see result 2.1 and definition 2.1. This is also physical: having occupation number zero for some 1-body state does not mean the state is $|\text{null}\rangle$. For the case $n_\alpha=0$, $\delta_{\alpha,\alpha'_j}$ is always zero, so the resulting state is $|\text{null}\rangle$. Physically, we *should not* be able to annihilate a particle in the state $|\alpha\rangle$ when there is nothing to be annihilated in the state $|\alpha\rangle$. That the RHS is $|\text{null}\rangle$ prohibits this absurd annihilation process, because anything that follows would be happening to $|\text{null}\rangle$ and therefore have no physical consequence. [9]

Although its expression seems complicated, the norm of $\hat{\psi}_\alpha\left|\alpha'_1,\dots,\alpha'_m\right\rangle$ is always $\sqrt{n_\alpha}$, because: If $n_\alpha=0$ then this quantity equals to zero, our claim is true. Otherwise, for bosons the n_α contributing terms are all identical, so the prefactor is

$$\frac{1}{\sqrt{n_\alpha}}\times n_\alpha=\sqrt{n_\alpha}.$$

For fermions n_α is 1 if not zero, so there is only one contributing term and the norm is simply

$$\frac{1}{\sqrt{1}}\times 1=1,$$

with the overall phase ζ^{j-1} which doesn't affect the vector's norm.

[8] When permuting the indices in the vestor, we are just re-labelling the summation index P.

[9] For all operators, $|\text{null}\rangle$ will be mapped to itself, and the expectation value under $|\text{null}\rangle$ is always zero.

Result 3.1. The operator $\hat{\psi}_\alpha$ maps the state $|\alpha'_1, \ldots, \alpha'_m\}$ to

$$\sum_{j=1}^{m} \zeta^{j-1} \delta_{\alpha,\alpha'_j} |\alpha'_1, \ldots, \alpha'_{j-1}, \alpha'_{j+1}, \ldots, \alpha'_m\},$$

which can be interpreted as the annihilation of a particle in the 1-body state $|\alpha\rangle$. For Fock states,

$$\hat{\psi}_\alpha |\alpha'_1, \ldots, \alpha'_m\rangle = \begin{cases} |\text{null}\rangle & \text{if } n_\alpha = 0, \\ n_\alpha^{-1/2} \sum_{j=1}^{m} \zeta^{j-1} \delta_{\alpha,\alpha'_j} |\alpha'_1, \ldots, \alpha'_{j-1}, \alpha'_{j+1}, \cdots, \alpha'_m\rangle & \text{if } n_\alpha \neq 0. \end{cases} \tag{3.2}$$

and

$$\left\| \hat{\psi}_\alpha |\alpha'_1, \ldots, \alpha'_m\rangle \right\| = \sqrt{n_\alpha}. \tag{3.3}$$

Remark 3.1. The prefactor ζ^{j-1} in eqn. (3.2) seems strange because it depends on the specific labelling of particles, while we have claimed Fock states and their properties to depend exclusively on occupation numbers. In fact this prefactor has very simple consequences. For bosons it is always 1, which is trivial. For fermions there can be at most one contributing term, so this prefactor is an overall phase. Recalling remark 2.3, we see that this overall phase arises from our choice of ordering convention of 1-body states when writing down $|\alpha'_1, \ldots, \alpha'_m\}$.

Remark 3.2. Here we have defined the creation and annihilation operators in terms of partially normalized states and *derived* their action on Fock states. There is another approach [2, § 2.1] which defines these operators in terms of how they act on Fock states. Had we used this approach, it would be hard to see how $\hat{\psi}_\alpha$ maps a quantum state where $n_\alpha = 0$ to the null vector, but in our approach this is a natural consequence.

Motivation 3.3. After creating and annihilating a particle in the 1-body state $|\alpha\rangle$, the occupation number n_α remains the same. Besides,

$$\left\| \hat{\psi}^\dagger_\alpha |\alpha'_1, \ldots, \alpha'_N\rangle \right\| = \sqrt{n_\alpha + 1}, \quad \left\| \hat{\psi}_\alpha |\alpha'_1, \ldots, \alpha'_N\rangle \right\| = \sqrt{n_\alpha},$$

so applying the creation and annihilation operators not only manipulates occupation numbers, but also adds overall scale factors $\sqrt{n_\alpha + 1}$, $\sqrt{n_\alpha}$. We are therefore motivated to use these scale factors to construct the number operator as mentioned in remark 2.1.

We want to obtain n_α by $\sqrt{n_\alpha} \times \sqrt{n_\alpha}$, but $\hat{\psi}^\dagger_\alpha$ is associated with $\sqrt{n_\alpha + 1}$. Hence we annihilate an operator first so that the scale factor associated with $\hat{\psi}^\dagger_\alpha$ becomes $\sqrt{n_\alpha}$; *i.e.* we try the operator $\hat{\psi}^\dagger \hat{\psi}$.

If $n_\alpha \neq 0$,

$$\begin{aligned} \hat{\psi}^\dagger \hat{\psi} |\alpha'_1, \ldots, \alpha'_N\rangle &= \hat{\psi}^\dagger \frac{1}{\sqrt{n_\alpha}} \sum_{j=1}^{d} \zeta^{j-1} \delta_{\alpha,\alpha'_j} |\alpha'_1, \ldots, \alpha'_{j-1}, \alpha'_{j+1}, \ldots, \alpha'_N\rangle \\ &= \frac{\sqrt{(n_\alpha - 1) + 1}}{\sqrt{n_\alpha}} \sum_{j=1}^{d} \zeta^{j-1} \delta_{\alpha,\alpha'_j} |\alpha\alpha'_1, \ldots, \alpha'_{j-1}, \alpha'_{j+1}, \ldots, \alpha'_N\rangle, \end{aligned}$$

but

$$\zeta^{j-1} \delta_{\alpha,\alpha'_j} |\alpha\alpha'_1, \ldots, \alpha'_{j-1}, \alpha'_{j+1}, \ldots, \alpha'_N\rangle = |\alpha'_1, \ldots, \alpha'_N\rangle$$

because $\delta_{\alpha,\alpha'_j}$ enforces $\alpha = \alpha'_j$, and permuting $|\alpha\rangle$ to the jth place cancels ζ^{j-1}. There are n_α identical contributing terms, hence

$$\hat{\psi}^\dagger_\alpha \hat{\psi}_\alpha |\alpha'_1, \ldots, \alpha'_N\rangle = n_\alpha |\alpha'_1, \ldots, \alpha'_N\rangle.$$

If $n_\alpha = 0$ then

$$\hat{\psi}_\alpha |\alpha'_1, \ldots, \alpha'_N\rangle = |\text{null}\rangle = 0 \times |\alpha'_1, \ldots, \alpha'_N\rangle,$$

and therefore the equation

$$\hat{\psi}_\alpha^\dagger \hat{\psi}_\alpha \left|\alpha_1', \ldots, \alpha_N'\right\rangle = n_\alpha \left|\alpha_1', \ldots, \alpha_N'\right\rangle$$

holds whatever n_α is.

The operator $\hat{\psi}^\dagger \hat{\psi}$ is Hermitian because

$$\left(\hat{\psi}^\dagger \hat{\psi}\right)^\dagger = \hat{\psi}^\dagger \left(\hat{\psi}^\dagger\right)^\dagger = \hat{\psi}^\dagger \psi.$$

Comparing $\hat{\psi}_\alpha^\dagger \hat{\psi}$ with what was required in remark 2.1, we see that it fits the definition.

Result 3.2. Associated to each 1-body state $|\alpha\rangle$ is a Hermitian number operator

$$\hat{n}_\alpha := \hat{\psi}_\alpha^\dagger \hat{\psi}_\alpha \tag{3.4}$$

which produces n_α when acting on a Fock state:

$$\hat{n}_\alpha \left|n_{\lambda_1}, \ldots, n_{\lambda_n}\right\rangle = n_\alpha \left|n_{\lambda_1}, \ldots, n_{\lambda_n}\right\rangle. \tag{3.5}$$

Summing over all occupation numbers gives the total particle number:

$$\sum_\alpha \hat{n}_\alpha \left|n_{\alpha_1}, \ldots, n_{\alpha_d}\right\rangle = N \tag{3.6}$$

with $\{|\alpha_j\rangle\}_{j=1}^d$ the 1-body basis and $N = \sum_{j=1}^d n_j$.

Motivation 3.4. As is customary for newly introduced operators, we study the commutators and how to swtich bases for the creation and annihilation operators. The formulas obtained below will be important tools for calculation.

First, we study the commutators between raising operators of different 1-body states $|\alpha\rangle, |\alpha'\rangle$.

$$\begin{aligned}
\hat{\psi}_\alpha^\dagger \hat{\psi}_{\alpha'}^\dagger |\alpha_1, \ldots, \alpha_n\} &= \hat{\psi}_\alpha^\dagger |\alpha' \alpha_1, \ldots, \alpha_n\} \\
&= |\alpha \alpha' \alpha_1, \ldots, \alpha_n\} \\
&= \zeta |\alpha' \alpha \alpha_1, \ldots, \alpha_n\} \\
&= \zeta \hat{\psi}_{\alpha'}^\dagger \hat{\psi}_\alpha^\dagger |\alpha_1, \ldots, \alpha_n\},
\end{aligned}$$

therefore

$$\left[\hat{\psi}_\alpha^\dagger, \hat{\psi}_{\alpha'}^\dagger\right]_{-\zeta} = 0,$$

where

$$\left[\hat{A}, \hat{B}\right]_{-\zeta} := \hat{A}\hat{B} - \zeta \hat{B}\hat{A}.$$

Similarly, $\left[\hat{\psi}_\alpha, \hat{\psi}_{\alpha'}\right]_{-\zeta} = 0.$

Next we study the commutator between creation and annihilation operators.

$$\begin{aligned}
\hat{\psi}_\alpha \hat{\psi}_{\alpha'}^\dagger |\alpha_1, \ldots, \alpha_n\} &= \hat{\psi}_\alpha |\alpha' \alpha_1, \ldots, \alpha_n\} \\
&= \delta_{\alpha,\alpha'} |\alpha_1, \ldots, \alpha_n\} + \sum_{j=2}^{n+1} \zeta^{j-1} \delta_{\alpha,\alpha_j} |\alpha' \alpha_1, \ldots, \alpha_{j-1}, \alpha_{j+1}, \ldots, \alpha_n\},
\end{aligned}$$

while applying them in the other order gives

$$\begin{aligned}
\hat{\psi}_{\alpha'}^\dagger \hat{\psi}_\alpha |\alpha_1, \ldots, \alpha_n\} &= \hat{\psi}_{\alpha'}^\dagger \sum_{j=1}^{n} \zeta^{j-1} \delta_{\alpha,\alpha_j} |\alpha_1, \ldots, \alpha_{j-1}, \alpha_{j+1}, \cdots, \alpha_n\} \\
&= \sum_{j=1}^{n} \zeta^{j-1} \delta_{\alpha,\alpha_j} |\alpha' \alpha_1 \cdots \alpha_{j-1}, \alpha_{j+1}, \ldots, \alpha_n\}.
\end{aligned}$$

It follows that

$$\left[\hat{\psi}_\alpha, \hat{\psi}^\dagger_{\alpha'}\right]_{-\zeta} = \delta_{\alpha,\alpha'}.$$

Result 3.3. For creation and annihilation operators,

$$\left[\hat{\psi}^\dagger_\alpha, \hat{\psi}^\dagger_{\alpha'}\right]_{-\zeta} = \left[\hat{\psi}_\alpha, \hat{\psi}_{\alpha'}\right]_{-\zeta} = 0 \tag{3.7}$$

$$\left[\hat{\psi}_\alpha, \hat{\psi}^\dagger_{\alpha'}\right]_{-\zeta} = \delta_{\alpha,\alpha'} \tag{3.8}$$

with

$$\left[\hat{A}, \hat{B}\right]_{-\zeta} := \hat{A}\hat{B} - \zeta\hat{B}\hat{A}. \tag{3.9}$$

Creation and annihilation operators of different modes always (anti)commute; operators of the same mode need more attention because their commutator might produce a kronecker delta.

The creation and annihilation operators are defined in terms of how they act on partially normalized state. Such states transform as

$$|\tilde{\alpha}\alpha_1 \cdots \alpha_n\} = \sum_\alpha \langle\alpha|\tilde{\alpha}\rangle \times |\alpha\alpha_1 \cdots \alpha_n\},$$

with $\{|\tilde{\alpha}\rangle\}$ and $\{|\alpha\rangle\}$ 1-body bases. Therefore

$$\begin{aligned} \hat{\psi}^\dagger_{\tilde{\alpha}}|\alpha_1 \cdots \alpha_n\} &= \sum_\alpha \langle\alpha|\tilde{\alpha}\rangle \times |\alpha\alpha_1, \ldots, \alpha_n\} \\ &= \sum_\alpha \langle\alpha|\tilde{\alpha}\rangle\, \hat{\psi}^\dagger_\alpha|\alpha_1 \cdots \alpha_n\}, \end{aligned}$$

from which it follows that

$$\hat{\psi}^\dagger_{\tilde{\alpha}} = \sum_\alpha \langle\alpha|\tilde{\alpha}\rangle\, \hat{\psi}^\dagger_\alpha.$$

Taking the Hermitian adjoint of this equation gives

$$\hat{\psi}_{\tilde{\alpha}} = \sum_\alpha \langle\tilde{\alpha}|\alpha\rangle\, \hat{\psi}_\alpha.$$

Result 3.4. Given the creation and annihilation operators under the 1-body basis $\{|\alpha\rangle\}$, switching to another 1-body basis $\{|\tilde{\alpha}\rangle\}$ leads to new creation and annihilation operators

$$\begin{aligned} \hat{\psi}^\dagger_{\tilde{\alpha}} &= \sum_\alpha \langle\alpha|\tilde{\alpha}\rangle\, \hat{\psi}^\dagger_\alpha \\ \hat{\psi}_{\tilde{\alpha}} &= \sum_\alpha \langle\alpha|\tilde{\alpha}\rangle^*\, \hat{\psi}_\alpha \end{aligned}$$

where the creation operator transforms like a vector (ket), and the annihilation operator transforms like a 1-form (bra). One may remember the formula for $\hat{\psi}^\dagger_{\tilde{\alpha}}$ easily by noting that immediately after writing down sum over α, the coefficient $\langle\alpha|\tilde{\alpha}\rangle$ begins with α.

Remark 3.3. Switching to an infinite-dimensional 1-body basis requires replacing the sum with integration and the Kronecker delta with Dirac delta. For example, consider the so-called field operator [10]

$$\hat{\psi}^\dagger(\mathbf{r}) := \sum_\alpha \langle\alpha|\mathbf{r}\rangle\, \hat{\psi}^\dagger_\alpha,$$

[10] Field operators are just creation and annihilation operators under the position basis.

its commutators involve Dirac (instead of Kronecker) delta functions:

$$\left[\hat{\psi}(\mathbf{r}), \hat{\psi}^\dagger(\mathbf{r}')\right] = \delta(\mathbf{r}-\mathbf{r}').$$

This is reasonable because when evaluating expectation values, these operators will be integrated over $\mathbf{r}$ and $\mathbf{r}'$, and the Dirac delta can pick up a finite value while the Kronecker delta cannot.

3.2 Analogy with the harmonic oscillator

This subsection can be skipped. It is included because many texts use the harmonic oscillator to motivate the definition of the creation and annihilation operators, which might cause confusion.

The quantum 1-dimensional harmonic oscillator with the Hamiltonian

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2 = \hbar\omega\left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\right)$$

has discrete energy eigenstates $\{|n\rangle\}_{n=0}^{\infty}$ related by the "ladder operators"

$$\hat{a}^\dagger = \sqrt{\frac{m\omega}{2\hbar}}\left(\hat{x} - \frac{\mathrm{i}}{m\omega}\hat{p}\right), \hat{a} = \sqrt{\frac{m\omega}{2\hbar}}\left(\hat{x} + \frac{\mathrm{i}}{m\omega}\hat{p}\right)$$

such that

$$\hat{a}^\dagger|n\rangle = \sqrt{n+1}\,|n+1\rangle\,, \hat{a}\,|n\rangle = \sqrt{n}\,|n-1\rangle\,.$$

From this point of view, the quantum harmonic oscillator can be viewed as a many-body system with the 1-body Hilbert space $\mathrm{span}\{|\mathrm{HO}\rangle\} = \mathbb{C}^1$. The ladder operators create or annihilate "particles" in the 1-body state $|\mathrm{HO}\rangle$.

Recall that for Fock states, each 1-body state $|\alpha\rangle$ corresponds to a pair of operators $\hat{\psi}_\alpha^\dagger$, $\hat{\psi}_\alpha$ which can create or annihilate a particle in $|\alpha\rangle$. To form an analogy with a many-body system with 1-body Hilbert space $\mathbb{C}^d$, we need d independent harmonic oscillators, with the wavefunction

$$|n_1, n_2, \ldots, n_d\rangle \coloneqq \bigotimes_{j=1}^{d} |n_j\rangle\,,$$

where each $|n_j\rangle$ labels the state of one harmonic oscillator. When the jth harmonic oscillator is excited by $\hat{a}_j^\dagger$, *i.e.* when the wavefunction $|n_1, n_2, \ldots, n_d\rangle$ is acted upon by this operator, we *think about this event as if* a boson is created in the 1-body state corresponding to the jth harmonic oscillator. This is the analogy with the harmonic oscillator; it arrives at the bosonic Fock state via a specific hamiltonian.

Had we introduced second quantization with this analogy, we would not be able to know whether the formalism depends on the harmonic oscillator in some fundamental way, or whether the second quantization for fermions can also be constructed with an analogy. Besides, the state $|\mathrm{HO}\rangle$ is totally abstract; we do not know what it is.

However, our discussions prior to this subsection were *altogether independent of any Hamiltonian.* It is clear from our approach that second quantization does not depend on the harmonic oscillator.

But this analogy does reveal that the harmonic oscillator is something special. In fact, the quantized electromagnetic field turns out to be a sum of harmonic oscillators whose excitations are photons.

4 Operators under second quantization

Motivation 4.1. The key difficulty is the conflict between our basis and the way we make sense of operators. We are only familiar with the way in which operators act on product states, but we are now using Fock states. To resolve this we project Fock states onto the product basis and act the operators on them. After that we collect the terms. The general recipe would be to act an operator on a "partially normalized state" and then abstract away the state [11] to obtain an operator equation.

[11] While not normalized, the basis $\{|\alpha_1, \ldots, \alpha_N\}\}$ is still an orthogonal and complete one.

4.1 1-body operators

By definition, a 1-body operator $\hat{V}$ visits the particles in a product state one by one. Under a basis where $\hat{V}$ is diagonal, *i.e.* within each 1-body space, $\hat{V} = \sum_{j=1}^{d} \lambda_j |\lambda_j\rangle \langle\lambda_j|$, acting it on a product state would produce

$$\begin{aligned}\hat{V}|\alpha_1, \ldots, \alpha_N) &= \sum_{i=1}^{N} \hat{V}^{(i)}|\alpha_1, \ldots, \alpha_N) \\ &= \sum_{i=1}^{N} \alpha_i|\alpha_1, \ldots, \alpha_N)\end{aligned}$$

where $\alpha_i \in \{\lambda_j\}$ and the superscript (i) on $\hat{V}$ indexes the 1-body space $\hat{V}$ acts on. Note that the sum $\sum_{i=1}^{N} \alpha_i$ only depends on occupation numbers, hence it is invariant upon permutation of particles.

Following the recipe mentioned in motivation 4.1 we calculate $\hat{V}|\alpha_1, \ldots, \alpha_N\}$,

$$\begin{aligned}\hat{V}|\alpha_1, \ldots, \alpha_N\} &= \frac{1}{\sqrt{N!}} \sum_P \zeta^{|P|} \hat{V}|\alpha_{P1}, \ldots, \alpha_{PN}\} \\ &= \frac{1}{\sqrt{N!}} \sum_P \zeta^{|P|} \sum_{i=1}^{N} \hat{V}^{(Pi)}|\alpha_{P1}, \ldots, \alpha_{PN}\} \\ &= \frac{1}{\sqrt{N!}} \sum_P \zeta^{|P|} \sum_{i=1}^{N} \alpha_{Pi}|\alpha_{P1}, \ldots, \alpha_{PN}\} \\ &= \frac{1}{\sqrt{N!}} \sum_P \zeta^{|P|} \left(\sum_{j=1}^{d} \hat{n}_{\lambda_j} \lambda_j \right) |\alpha_{P1}, \ldots, \alpha_{PN}\} \\ &= \sum_{j=1}^{d} \hat{n}_{\lambda_j} \lambda_j |\alpha_1, \ldots, \alpha_N\},\end{aligned}$$

where the last equality holds because in the second-to-last line, the term $\sum_j \hat{n}_j \lambda_j$ is independent of P and thus can be factorized.

Switching basis should follow from straightforward calculation: start with

$$\hat{V}^{(1)} = \sum_{j=1}^{d} \langle j| \hat{V} |j\rangle \hat{\psi}_j^\dagger \hat{\psi}_j,$$

where we have denoted $|\lambda_j\rangle$ with $|j\rangle$, and insert

$$\hat{\psi}_j^\dagger = \sum_{i'} \langle i'|j\rangle \hat{\psi}_{i'}^\dagger, \quad \hat{\psi}_j = \sum_{k'} \langle k'|j\rangle^* \hat{\psi}_{k'}$$

to obtain

$$\begin{aligned}\hat{V}^{(1)} &= \sum_{j,i',k'} \langle j| \hat{V} |j\rangle \hat{\psi}_{i'}^\dagger \hat{\psi}_{k'} \langle i'|j\rangle \langle j|k'\rangle \\ &= \sum_{j,i',k'} \langle i'|j\rangle \langle j| \hat{V} |j\rangle \langle j|k'\rangle \hat{\psi}_{i'}^\dagger \hat{\psi}_{k'} \\ &= \sum_{i',k'} \langle i'| \hat{V} |k'\rangle \hat{\psi}_{i'}^\dagger \hat{\psi}_{k'},\end{aligned}$$

where the last equation holds because summing over j in $|j\rangle \langle j|$ produces $\mathbb{1}$.

Result 4.1. Under second quantization, a 1-body operator $\hat{V}$ takes the form of

$$\hat{V} = \sum_{i,j=1}^{d} \hat{\psi}^\dagger_{\lambda_i} \hat{\psi}_{\lambda_j} \langle\lambda_i| \hat{V} |\lambda_j\rangle \,, \tag{4.1}$$

where $\{|\lambda_j\rangle\}_{j=1}^d$ is any basis for the 1-body Hilbert space $\mathbb{C}^d$. If $\{|\lambda_j\rangle\}$ is an eigenbasis of $\hat{V}$ then we can insert $i = j$ and sum over i.

Remark 4.1. From the calculations that led to result 4.1, we can see the general recipe of deriving operators under second quantization:

1. Because $\hat{V}$ acting on a product state produces a scalar $\sum_i \alpha_i$ that is independent of permutation, this scalar can be factorized out of the sum over permutations.
2. Because $\forall\ f : \mathbb{C}^d \mapsto \mathbb{C}$ and a Fock state $|\alpha_1, \ldots, \alpha_N\rangle$ with 1-body Hilbert space $\mathbb{C}^d$ we have

$$\sum_{i=1}^{N} f(|\alpha_i\rangle) = \sum_{j=1}^{d} n_{\lambda_j} f(|\lambda_j\rangle),$$

we can express $\hat{V}$ in terms of the number operator.

Remark 4.2. The only information carried by a physical state is occupation numbers, so it is only natural that any Hermitian operator can be expressed in terms of number operators.

4.2 2-body operators

By definition, 2-body operators act on *pairs* of particles only. For a 2-body operator $\hat{U}$, under its eigenbasis $\{|\lambda_j\rangle\}_{j=1}^d$, $\hat{U} = \sum_{p<q} \hat{U}^{(p,q)}$ where

$$\hat{U}^{(p,q)} = \hat{U}^{(p)} \otimes \hat{U}^{(q)}$$

with 1-body operators $\hat{U}^{(p)} = \hat{U}^{(q)} = \sum_{j=1}^d \lambda_j |\lambda_j\rangle \langle\lambda_j|$.

Therefore, acting $\hat{U}$ on a product state gives

$$\begin{aligned}\hat{U}|\alpha_1, \ldots, \alpha_N) &= \sum_{i<j} \hat{U}^{(i,j)} |\alpha_1, \ldots, \alpha_N) \\ &= \sum_{i<j} \alpha_i \alpha_j |\alpha_1, \ldots, \alpha_N)\end{aligned}$$

with $\alpha_i, \alpha_j \in \{\lambda_k\}_{k=1}^d$.

We apply the recipe given in remark 4.1,

1. Factorizing the scalar,

$$\begin{aligned}\hat{U}|\alpha_1, \ldots, \alpha_N\} &= \frac{1}{\sqrt{N!}} \sum_P \zeta^{|P|} \hat{U} |\alpha_{P1}, \ldots, \alpha_{PN}) \\ &= \left(\sum_{i<j} \alpha_i \alpha_j \right) |\alpha_1, \ldots, \alpha_N\},\end{aligned}$$

2. Expressing the scalar in terms of occupation numbers,

$$
\begin{aligned}
\sum_{i<j} \alpha_i \alpha_j &= \frac{1}{2}\left(\sum_{i,j=1}^{N} - \sum_{i=j}\right) \alpha_i \alpha_j \\
&= \frac{1}{2}(\sum_i \alpha_i)(\sum_j \alpha_j) - \frac{1}{2}\sum_i \alpha_i^2 \\
&= \frac{1}{2}\sum_{\lambda,\lambda'} \lambda\lambda' n_\lambda n_{\lambda'} - \frac{1}{2}\sum_\lambda n_\lambda \lambda^2 \\
&= \frac{1}{2}\sum_{\lambda,\lambda'} \lambda\lambda'(n_\lambda n_{\lambda'} - \delta_{\lambda,\lambda'} n_\lambda),
\end{aligned}
$$

where λ, λ' label 1-body eigenvalues,

to obtain the second-quantized formula for 2-body operators,

$$
\hat{U} = \frac{1}{2}\sum_{\lambda,\lambda'} \lambda\lambda' \left(\hat{n}_\lambda \hat{n}_{\lambda'} - \delta_{\lambda,\lambda'} \hat{n}_\lambda\right).
$$

In fact, $\hat{n}_\alpha \hat{n}_\beta - \delta_{\alpha,\beta}\hat{n}_\alpha$ equals to $\hat{\psi}^\dagger_\alpha \hat{\psi}^\dagger_\beta \hat{\psi}_\beta \hat{\psi}_\alpha$. If $\alpha \neq \beta$ then this equation is trivial; otherwise, we can verify this using result 3.3: for Bosons,

$$
\psi^\dagger\psi\psi^\dagger\psi - \psi^\dagger\psi = \psi^\dagger(\psi\psi^\dagger - \mathbb{1})\psi = \psi^\dagger\psi^\dagger\psi\psi,
$$

and for fermions $\psi^\dagger\psi^\dagger\psi\psi = 0$, while

$$
\psi^\dagger\psi\psi^\dagger\psi - \psi^\dagger\psi = \psi^\dagger(\psi\psi^\dagger - \mathbb{1})\psi = -\psi^\dagger\psi^\dagger\psi\psi = 0.
$$

Therefore, under second quantization, a 2-body operator $\hat{U}$ is

$$
\hat{U} = \frac{1}{2}\sum_{\lambda,\lambda'} (\lambda\lambda'|\hat{U}|\lambda\lambda')\hat{\psi}^\dagger_\lambda \hat{\psi}^\dagger_{\lambda'} \hat{\psi}_{\lambda'} \hat{\psi}_\lambda.
$$

Concerning switching basis, if we take the straightforward approach of inserting the transformation for $\hat{\psi}^\dagger_\lambda$, $\hat{\psi}^\dagger_{\lambda'}$, $\hat{\psi}_{\lambda'}, \hat{\psi}_\lambda$, then the calculation would be tedious. Instead we reduce the problem at hand to one already solved: switching basis for 1-body operators. In eqn. (4.1) the basis is *arbitrary*, meaning that this equation is formally basis independent. If we can write down 2-body operators in terms of that equation, then their expression become formally basis independent, too.

We now re-write $\hat{U}$ in terms of 1-body operators. Recalling $\hat{U}$ is a sum of terms like $\hat{U}^{(p)} \otimes \hat{U}^{(q)}$, the inner product $(\lambda\lambda'|\hat{U}|\lambda\lambda')$ is just a sum of terms like

$$
\begin{aligned}
(\lambda\lambda'|\hat{U}^{(p)} \otimes \hat{U}^{(q)}|\lambda\lambda') &= (\lambda\lambda'|\hat{U}^{(p)} \otimes \mathbb{1}^{(q)}|\lambda\lambda') \times (\lambda\lambda'|\mathbb{1}^{(p)} \otimes \hat{U}^{(q)}|\lambda\lambda') \\
&= \langle\lambda|\,\hat{U}^{(p)}\,|\lambda\rangle \times \langle\lambda'|\,\hat{U}^{(q)}\,|\lambda'\rangle\,,
\end{aligned}
$$

which are 1-body quantities.

Having taken care of the scalar part $(\lambda\lambda'|\hat{U}|\lambda\lambda')$, let us examine the operator part of $\hat{U}$. In the equation

$$
\hat{U} = \frac{1}{2}\sum_{\lambda,\lambda'} \lambda\lambda' \left(\hat{n}_\lambda \hat{n}_{\lambda'} - \delta_{\lambda,\lambda'} \hat{n}_\lambda\right).
$$

there are two terms: the first one is

$$
(\lambda\lambda'|\hat{U}|\lambda\lambda')\hat{n}_\lambda \hat{n}_{\lambda'} = \langle\lambda|\,\hat{U}^{(p)}\,|\lambda\rangle\,\hat{n}_\lambda \times \langle\lambda'|\,\hat{U}^{(q)}\,|\lambda'\rangle\,\hat{n}_{\lambda'},
$$

and the second is zero for $\lambda \neq \lambda'$,

$$\langle\lambda|\,\hat{U}^{(p)}\,|\lambda\rangle\,\langle\lambda|\,\hat{U}^{(q)}\,|\lambda\rangle\,\hat{n}_\lambda = \langle\lambda|\Big(\hat{U}^{(1)}\Big)^2|\lambda\rangle\,\hat{n}_\lambda$$

for $\lambda = \lambda'$ where $\hat{U}^{(p)} = \hat{U}^{(q)} = \hat{U}^{(1)}$. Both terms consist of 1-body number operators multiplied by their corresponding eigenvalues, which match the form of eqn. (4.1), so they are formally basis independent.

Result 4.2. Under second quantization, a 2-body operator $\hat{U}$ is

$$\hat{U} = \frac{1}{2}\sum_{\alpha,\beta,\alpha',\beta'}^{d}(\alpha\beta|\hat{U}|\alpha'\beta')\hat{\psi}^\dagger_\alpha\hat{\psi}^\dagger_\beta\hat{\psi}_{\beta'}\hat{\psi}_{\alpha'}, \tag{4.2}$$

with $|\alpha\rangle, |\beta\rangle, |\alpha'\rangle, |\beta'\rangle \in \{|\lambda\rangle\}$, an arbitrary basis for the 1-body space $\mathbb{C}^d$. If $\{|\alpha\beta)\}$ is an eigenbasis of $\hat{U}$, then we can insert $\alpha = \alpha', \beta = \beta'$ and sum over α, β.

5 General comments and bibliographical notes

While important for any advanced study in physics, second quantization has not been given the rigor and emphasis it deserves in many texts. Most textbooks simply use the harmonic oscillator to motivate the formulae of creation and annihilation operators, and force the reader to accept Fock states without explicitly constructing them using product states.

The approach taken in this note is better than most books since it shows that second quantization is simply a basis transformation within physical subspaces from product states to Fock states (which are "scrambled" product states). There is hardly any physical subtlety or postulate related with second quantization, except perhaps that the physical nature of "permutation" depends on dimensionality, which gives rise to anyons in (2+1)D. [12]

This note treats the topic so that "by segregating mathematical theorems from physical postulates, any confusion as to which is which is nipped in the bud" [4]. While not particularly enthusiastic about formal topics in physics, I find this slightly formal introduction to second quantization suitable.

References

1. Dupuis, N. *Field theory of condensed matter and ultracold gases: Volume 1* 689 pp. ISBN: 978-1-80061-390-4 (World Scientific, 2023).
2. Altland, A. & Simons, B. *Condensed Matter Field Theory* 3rd ed. ISBN: 978-1-108-49460-1 (Cambridge University Press, 2023).
3. Simon, S. *Topological quantum* ISBN: 978-0-19-888672-3. `https://www-thphys.physics.ox.ac.uk/people/SteveSimon/topological2020/TopoBookOct27hyperlink.pdf` (Oxford University Press, New York, 2023).
4. Shankar, R. *Principles of Quantum Mechanics* ISBN: 978-1-4757-0578-2 978-1-4757-0576-8 (Springer US, New York, NY, 1994).

[12] A simple argument concerning how particle exchange statistics are fundamentally different between (2+1)D and (3+1)D can be found in Chapter 3 of [3]. Click on the hyperlink provided in the bibliography to access the free version of the book.