Advanced quantum mechanics (20104301)

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Chapter 3: Elements of second quantization

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3.1 Preliminary remarks

We have seen that the basis vectors of a system of N identical particles is completely described by the occupation numbers $(N_1, N_2, \dots)$. These occupation numbers tell us how many particles are in each single-particle mode, and this is all that is needed to capture the basis state. We can hence write the basis vectors in the simple form

$$|N_1, N_2, \dots\rangle. \tag{3.1}$$

In this context, it is helpful to grasp systems with the help of creation and annihilation operators. This is a concept rather familiar from the first course of quantum theory. We will nevertheless repeat it here and go in more depth.

3.2 Second quantization for bosons

Somewhat pedantically, we will introduce the *Fock space*: This separable Hilbert space is the direct sum of Hilbert spaces of fixed particle number, that is

$$\mathcal{H} = \bigoplus_{N=0}^{\infty} \mathcal{H}_{(N)}, \tag{3.2}$$

where $\mathcal{H}_{(N)}$, $N \geq 1$, is the Hilbert space of physically realizable pure states of N bosonic particles. $\mathcal{H}_{(0)} = \mathbb{C}$ is the one-dimensional vector space spanned by $|\o\rangle$, the vacuum state vector. Note that in the literature it is common to call both the space the Fock space as well as the one that is spanned by the vector of a fixed occupation number. Let us not get too much hung up and rather stress the occupation number basis for bosons.

Occupation numbers for bosons: The vectors

$$\mathcal{B} = \{|N_1, N_2, \dots\rangle : N_j \in \mathbb{N}_0, j = 1, 2, \dots\} \tag{3.3}$$

form a basis of the Hilbert space of identical bosons.

This basis is orthonormal and complete, in that

$$\langle N_1', N_2', \dots | N_1, N_2, \dots\rangle = \delta_{N_1', N_1}\delta_{N_2', N_2} \dots, \tag{3.4}$$

$$\sum_{N_1, N_2, \dots} |N_1, N_2, \dots\rangle\langle N_1, N_2, \dots| = \mathbb{1}. \tag{3.5}$$

Let us define now the annihilation operator, which we have already encountered when discussing the harmonic oscillator in the first course.

Annihilation operator for bosons: The *annihilation operator* for mode j is an operator in $\mathcal{H}$, for which

$$b_j|N_1, \dots, N_j, \dots\rangle = \sqrt{N_j}|N_1, \dots, N_j - 1, \dots\rangle \tag{3.6}$$

holds.

The– admittedly somehat unpleasant – name of the annihilation operator makes a lot of sense: It suggests to remove a particle in mode labeled j. We know immediately that

$$b_j|0, 0, \dots\rangle = b_j|\varnothing\rangle = 0. \tag{3.7}$$

Note also that $|\varnothing\rangle$ is not the null vector of the vector space. In the same way, we get via looking at the adjoint the following expression that we dedicate a box to only because we will so frequently make use of in the latter.

Creation operators for bosons: A *creation operator* for mode j is an operator in $\mathcal{H}$ for which

$$b_j^\dagger|N_1, \dots, N_j, \dots\rangle = \sqrt{N_j + 1}|N_1, \dots, N_j + 1, \dots\rangle. \tag{3.8}$$

In a bit of an inflation of boxes we will consider the following important operator, labeling the particle number in a given orbital or a mode:

Number operator for bosons: The operator $n_j = b_j^\dagger b_j$ with action

$$n_j^\dagger |N_1, \ldots, N_j, \ldots\rangle = N_j |N_1, \ldots, N_j, \ldots\rangle \tag{3.9}$$

is called *number operator*.

It will happen that we give operators hats, yet most often not to render the notation not unnecessarily clumsy. It should be clear at this point, however, that n_j is an operator in $\mathcal{H}$ and not only a number, unlike N_j. The *total particle number operator* is the operator

$$\sum_{j=1}^{N} n_j. \tag{3.10}$$

A system in a state with exactly N particles will hence will give rise to an expectation value N for the total particle number operator. Obviously, the spectrum of this operator is that of the non-negative numbers. It follows from the above definitions that bosonic operators fulfil the following commutation relations.

Bosonic commutation relations: The bosonic creation and annihilation operators satisfy

$$[b_j, b_k^\dagger] \quad = \quad \delta_{j,k}, \tag{3.11}$$

and

$$[b_j, b_k] = [b_j^\dagger, b_k^\dagger] = 0. \tag{3.12}$$

As usual, for pairs of operators, the *commutator* is defined as

$$[A, B] = AB - BA. \tag{3.13}$$

It is not uncommon to the define the *position* and *momentum operators*

$$x_j \quad = \quad (b_j + b_j)/\sqrt{2}, \tag{3.14}$$

$$p_j \quad = \quad i(b_j - b_j)/\sqrt{2} \tag{3.15}$$

We find immediately

$$|N_1, N_2, \ldots\rangle = (N_1! N_2! \ldots)^{-1/2} (b_1^\dagger)^{N_1} (b_2^\dagger)^{N_2} \ldots |\emptyset\rangle. \tag{3.16}$$

The precise order of definitions and corollaries are not consistent in text books on the subject. It should be clear that the bosonic commutation relations – the rules that define the *bosonic algebra* – are already defined via the above rules and give rise to the bosonic operators up to a phase. We could have introduce first the bosonic commutation relations and would have ended up in the occupation number representation.[1]

[1]Let us here see how we can derive the occupation number representation from the bosonic commutation

3.3 Second quantization for fermions

3.3.1 Creation and annihilation operators for fermions

Let us start by defining the annihilation and creation operators for fermions. They are defined as follows.

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relations. We are somewhat innocent here, but it should be clear that this can be made fully rigorous: We will present the argument for one orbital or mode that is hence no longer necessary. Let us hence look at an operator b for which $[b, b^\dagger] = 1$ holds. $b^\dagger b$ is also a Hermitian and positive operator. Its spectrum must therefore be included in the non-negative real numbers. Let us now consider

$$[b^\dagger b, b] = -b. \tag{3.17}$$

From Eq. (3.17) it follows that b applied to an eigenvector of $b^\dagger b$ of eigenvalue N again delivers an eigenvector, the eigenvalue of which is reduced by 1,

$$\begin{aligned} b^\dagger b(b|N\rangle) &= b(b^\dagger b)|N\rangle + [b^\dagger b, b]|N\rangle \\ &= (N-1)(b|N\rangle). \end{aligned} \tag{3.18}$$

Iterated application of this rule must lead to a zero eigenvalue. Otherwise, we would arrive at a contradiction with the observation that $b^\dagger b$ is a positive operator. Hence 0 must be a (and the smallest) eigenvalue of the number operator. In the same way, we find

$$[b^\dagger b, b^\dagger] = b^\dagger, \tag{3.19}$$

so that $b^\dagger$ is a creation operator that increases the eigenvalue of the number operator by 1. Hence, we arrive at the conclusion that the spectrum of $b^\dagger b$ are exactly the non-negative integers with eigenvectors $\{|N\rangle\}$. Similarly,

$$b|N\rangle = N^{1/2}|N-1\rangle, \tag{3.20}$$

$$b^\dagger|N\rangle = (N+1)^{1/2}|N+1\rangle, \tag{3.21}$$

up to a global phase factor. This is actually the only freedom we have here, and without loss of generality, we can set the phase to zero, since

$$\langle N|b^\dagger b|N\rangle = N. \tag{3.22}$$

The same argument can be applied to a multi-mode system, simply by adding a label j to the respective operators, and noting that operators acting on different modes must commute. Slightly more precisely put, the core question is whether every irreducible representation reflecting (3.11) und (3.12) is unitary equivalent to the Fock representation. There are some technicalities coming into play here, arising from the observation that the operators b_j and $b_j^\dagger$ are unbounded. For this reason, in mathematical physics, the commutation relations are usually not defined directly in terms of b_j und $b_j^\dagger$, but for their exponentiated form, the so-called *Weyl operators*. In this framework one indeed encounters under the additional assumption of the existence of a vacuum a unique Fock representation up to a phase.

Annihilation and creation operators for fermions: An *annihilation operator* for mode j is an operator, for which

$$f_j|N_1,\dots,N_j,\dots\rangle = (-1)^{\sum_{k=1}^{j-1} N_k} N_j |N_1,\dots,1-N_j,\dots\rangle \tag{3.23}$$

holds true, where now $N_j \in \{0,1\}$. For this reason, the *fermionic creation operator* satisfies

$$f_j^\dagger|N_1,\dots,N_j,\dots\rangle = (-1)^{\sum_{k=1}^{j-1} N_k}(1-N_j)|N_1,\dots,1-N_j\dots\rangle. \tag{3.24}$$

As before, the vacuum $|\emptyset\rangle$ is mapped by all f_j onto the null vector. Again, the – now fermionic – *number operator*

$$n_j = f_j^\dagger f_j \tag{3.25}$$

has the same role and is given the same name as the equivalent of a bosonic operator. These are the familiar laws as they originate from the *fermionic anticommutation relations*. Such anticommutation rules are given for pairs of operators as

$$\{A,B\} = AB + BA. \tag{3.26}$$

Anticommutation relations for fermionic operators: For fermionic creation and annihilation operators, the following familiar anticommutation rules hold true,

$$\{f_j, f_k^\dagger\} = \delta_{j,k}, \tag{3.27}$$

$$\{f_j, f_k\} = \{f_j^\dagger, f_k^\dagger\} = 0. \tag{3.28}$$

As before, we also find the analogous occupation number expressions for fermions.

Occupation numbers for fermions: The vectors

$$\mathcal{B} = \{|N_1,\dots,N_j,\dots\rangle = (f_1^\dagger)^{N_1}\dots(f_j^\dagger)^{N_j}\dots|\emptyset\rangle,\; N_1,N_2,\dots\in\{0,1\}\} \tag{3.29}$$

form a basis of the basis of identical fermions.

Basically all of the above expressions are still valid, but with replacing the commutation relations by anticommutation relations.[2]

[2]The Fock representation is, by the way, again unique and defined essentially by the anticommutation relation, if we postulate the existence of a vacuum and a fully occupied state.

3.3.2 Causality, superselection rules and Majorana fermions

Familiar? Wait a second. Eq. (3.23) contains the innocent looking phase

$$(-1)^{\sum_{k=1}^{j-1} N_k} \tag{3.30}$$

that contains all the particle numbers N_k of the modes to the "left" of orbital labeled j. This expression might be surprising and confusing in more than one way:

- On the one hand, this expression depends on the *order* of fermions. But this order is obviously completely up to us. Our predictions of physical properties must not depend on how we order modes in our description.

- More disturbing is the property that one could in principle observe this phase, leading to a fierce violation of causality.

The latter is compelling: it is easy to see that one can generate situations involving three modes, one, say, on Mars and two kept on Earth. Then the measurement of an operator that involves an odd number of fermionic annihilation and creation operators reveals by a phase whether a particle is present at Mars or not. But in this way, one can do instantaneous communication, faster than light: One merely has to place a particle in the mode on Mars or not. Such *superluminal communication* is not allowed in physics.

The resolution of this apparent dilemma is one that is stated in surprisingly few text books, even though this issue often gives rise to confusion. In fact, the resolution is that not all observables are allowed for fermionic operators. But only those that respect the *superselection rule* of the parity of fermion number. Any legitimate fermionic operator must commute with the parity operator The *parity operator* can be written as

$$P = i^N \prod_{j=1}^{2N} c_j \tag{3.31}$$

in terms of the $2N$ *Majorana fermions*.

Majorana fermions: The Majorana fermions of N fermionic modes are defined as

$$c_{2j-1} = f_j^\dagger + f_j, \tag{3.32}$$
$$c_{2j} = (-i)(f_j^\dagger - f_j) \tag{3.33}$$

for $j = 1, \ldots, N$. They are Hermitian, $c_j = c_j^\dagger$ and fulfil the fermionic anticommutation relations

$$\{c_j, c_k\} = \delta_{j,k} \tag{3.34}$$

for $j, k = 1, \ldots, 2N$.

These Majorana fermions are "half fermions" and are exciting in their own right. They can be prepared in mesoscopic structures, showing topological features. We will get back to that later in the course. In other words, the Hilbert space can be decomposed into a direct sum

$$\mathcal{H} = \mathcal{H}_{\text{even}} \oplus \mathcal{H}_{\text{odd}}, \tag{3.35}$$

involving terms containing an even and an odd number of fermions, respectively. No physical interaction can mix the two terms and respects this direct sum. Again, without this rule one can easily construct paradoxa of the above type.[3] Obviously, for fermionic annihilation operators, we always have

$$(f_j^\dagger)^2 = 0, \tag{3.36}$$

as a manifestation of the fact that no two fermions can occupy the same orbital.

3.3.3 Single-body density operators and Pauli principles

As a final remark, we briefly mention single-body density operators for fermionic systems of n modes and N particles. For n fermionic modes and a state ρ, we can look at the $n \times n$ matrix C with entries

$$C_{j,k} = \text{tr}(f_j^\dagger f_k \rho)/N. \tag{3.37}$$

This is basically a correlation function. We easily find its properties. It is Hermitian by definition, so that

$$C = C^\dagger. \tag{3.38}$$

We also find that it is positive semi-definite. This is slightly less obvious, but can be seen by making a suitable fermionic mode transformation, so that

$$C \geq 0, \tag{3.39}$$

which means that the real eigenvalues of C are non-negative. Also

$$\text{tr}(C) = 1. \tag{3.40}$$

That is to say, C has precisely the properties of a density operator. For this reason, it is called *one-body density operator*. It is no density operator as a quantum state, of course. But it captures the correlation structure of a fermionic system in a correlation matrix that takes the form of a density operator. The familiar *Pauli principle* can now be stated that the eigenvalues $\lambda_1, \ldots, \lambda_n$ satisfy

$$0 \leq \lambda_j \leq 1. \tag{3.41}$$

This reflects the fact that in each mode, there must be at least zero and at most one fermions. It originates from the antisymmetry of the wave function of identical fermionic

[3]There is no bosonic equivalent of the parity of fermion number. For massless bosons, such as photons, one can perfectly well create superpositions of particle numbers. For example, state vectors of the form $(|0\rangle + |1\rangle)/\sqrt{2}$ can be prepared. Only if the particle have mass, the *mass superselection rule* applies, and again no superposition is possible. Massive bosonic particles can hence not be prepared in a superposition of different particle numbers.

particles. However, there are more constraints arising from the antisymmetry. There is an entire family of *generalized Pauli principles*: These are general constraints any one-body density operator must satisfy. They take the form of a simplex of the eigenvalues $\lambda_1, \ldots, \lambda_n$ of C. It is interesting to see that these constraints can be completely characterized. It is also worth stressing that the *stability of matter* is essentially a consequence of the Pauli principle, and not of interactions.