Advanced quantum mechanics (20104301)
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Chapter 4: Field operators

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Field operators

4.1 Definition of field operators

4.1.1 Bosonic field operators

We will now get back to bosonic systems; in fact, for some courses to come, we will to an extent oscillate between looking at bosonic and fermionic many-body systems. Let us start from noting that the one-body basis can be chosen arbitrarily in principle. When going from one set of bosonic operators to a new set, reflecting a basis transformation of this kind, this can be captured by a transformation

$$b_{g_j} = \sum_{k=1}^{\infty} \langle g_j | \psi_k \rangle b_k, \tag{4.1}$$

$$b_{g_j}^{\dagger} = \sum_{k=1}^{\infty} \langle \psi_k | g_j \rangle b_k^{\dagger}, \tag{4.2}$$

defined by the scalar product between single particle state vectors. Going to a picture of field operators can be seen as a transformation of this kind. They are very much helpful. On a higher level, the situation at hand is as follows: In second quantization, one merely states how many bosons are occupying what single-particle orbital. When we would like to find out how Hamiltonian interactions defined in the position representation manifest themselves, we would like to have some contact with the single-particle wave functions. This connection is delivered by the field operators. Without such field operators, it would not be obvious how to derive a Hamiltonian in second quantization in terms of bosonic creation and annihilation operators. They often serve the purpose of a vehicle: At the end of the day, the Hamiltonian does not necessarily contain the field operators any more, but they are helpful to get the right expressions in the first place. They are so important that they deserve a box.

Field operators: The *bosonic field operators* are defined as

$$b_j = \int d\xi \psi_j^*(\xi)\Psi(\xi), \quad b_j^\dagger = \int d\xi \psi_j(\xi)\Psi^\dagger(\xi), \tag{4.3}$$

conversely,

$$\Psi(\xi) = \sum_j \psi_j(\xi) b_j, \quad \Psi^\dagger(\xi) = \sum_j \Psi_j^*(\xi) b_j^\dagger, \tag{4.4}$$

and satisfy

$$[\Psi(\xi), \Psi(\xi')] = [\Psi^\dagger(\xi), \Psi^\dagger(\xi')] = 0, \tag{4.5}$$

as well as

$$[\Psi(\xi), \Psi^\dagger(\xi')] = \delta(\xi - \xi'). \tag{4.6}$$

We can write state vectors in terms of field operators as follows. If this looks a bit odd at first, please be patient, it will be used to formulate Hamiltonians of interacting models in a neat form, and again, to relate the wave functions in the position representation to a second quantized picture.

State vectors in terms of field operators: A general symmetrized state vector $|\psi_N\rangle$ of N particles can be written as

$$|\psi_N\rangle = \frac{1}{\sqrt{N!}} \int d\xi_1 \dots d\xi_N \psi_N(\xi_1, \dots, \xi_N) \Psi^\dagger(\xi_N) \dots \Psi^\dagger(\xi_1)|\varnothing\rangle. \tag{4.7}$$

The normalization of the state vectors follows from the symmetrized wave function. We hence start from the vacuum that we successively fill up, first by placing a particle at ξ_1 by means of $\Psi^\dagger(\xi_1)$, then with a particle at ξ_2 using $\Psi^\dagger(\xi_2)$ and so on. The wave function ψ_N specifies the amplitude of the respective term. Since the wave function is symmetrized, we have for bosonic wave functions of identical particles

$$\psi_N(\xi_1, \dots, \xi_N) = \psi_N(\xi_N, \dots, \xi_1) \tag{4.8}$$

and analogously for any other permutation of the coordinates, since these expression deliver identical expressions under symmetrization. We now turn to an interesting expression. The following is true.

Action of field operators on state vectors: When applying a bosonic field operator to a state vector, we get

$$\Psi(\xi)|\psi_N\rangle = \sqrt{N}\int d\xi_1 \dots d\xi_{N-1}\psi_N(\xi_1,\dots,\xi_{N-1},\xi)\Psi^\dagger(\xi_{N-1})\dots\Psi^\dagger(\xi_1)|\varnothing\rangle. \tag{4.9}$$

This expression will be helpful in a moment. We would like to derive this formula for two particles at first, then it will become clear how to obtain general expressions of this type. We have

$$|\psi_2\rangle = \frac{1}{\sqrt{2}}\int d\xi_1 d\xi_2 \psi_S(\xi_1,\xi_2)\Psi^\dagger(\xi_1)\Psi^\dagger(\xi_2)|\varnothing\rangle. \tag{4.10}$$

Therefore, making use of the commutation relations for bosonic field operators, we get

$$\begin{aligned}\Psi(\xi)|\psi_2\rangle &= \frac{1}{\sqrt{2}}\int d\xi_1 d\xi_2 \psi_2(\xi_1,\xi_2)\Psi(\xi)\Psi^\dagger(\xi_1)\Psi^\dagger(\xi_2)|\varnothing\rangle \\ &= \frac{1}{\sqrt{2}}\int d\xi_1 d\xi_2 \psi_2(\xi_1,\xi_2)\Psi^\dagger(\xi_1)\Psi(\xi)\Psi^\dagger(\xi_2)|\varnothing\rangle \\ &+ \frac{1}{\sqrt{2}}\int d\xi_2 \psi_2(\xi,\xi_2)\Psi^\dagger(\xi_2)|\varnothing\rangle \\ &= \frac{1}{\sqrt{2}}\int d\xi_1 d\xi_2 \psi_2(\xi_1,\xi_2)\Psi^\dagger(\xi_1)\Psi^\dagger(\xi_2)\Psi(\xi)|\varnothing\rangle \\ &+ \frac{1}{\sqrt{2}}\int d\xi_1 \psi_2(\xi_1,\xi)\Psi^\dagger(\xi_1)|\varnothing\rangle \\ &+ \frac{1}{\sqrt{2}}\int d\xi_2 \psi_2(\xi,\xi_2)\Psi^\dagger(\xi_2)|\varnothing\rangle. \end{aligned} \tag{4.11}$$

Since now $\psi_2(\xi_1,\xi) = \psi_2(\xi,\xi_1)$ for all ξ and ξ_1, since this function is symetric, and since

$$\Psi(\xi)|\varnothing\rangle = 0 \tag{4.12}$$

for all ξ, because annihilation operators acting on the vacuum always lead to the zero vector, we have

$$\Psi(\xi)|\psi_2\rangle = \sqrt{2}\int d\xi_1 \psi_2(\xi_1,\xi)\Psi^\dagger(\xi_1)|\varnothing\rangle. \tag{4.13}$$

For wave functions in the position representation we arrive at

$$(\Psi(\xi)\psi_2)(\xi_1) = \sqrt{2}\psi_2(\xi_1,\xi). \tag{4.14}$$

We can argue in a similar fashion for N particles: This is left to the reader as an exercise. But the idea should be clear: We again can exhange neighbouring terms iteratively.

4.1.2 Fermionic field operators

For fermionic field operators there is not so much left to say. Let us briefly state the anticommutation relations for fermionic field operators, when the coordinates are $\xi = (x, \sigma)$, as position and a third spin component.

Fermionic field operators: The *fermionic field operators* fulfill the anticommutation relations

$$\{\Psi(x,\sigma), \Psi^\dagger(x',\sigma')\} = \delta(x-x')\delta_{\sigma,\sigma'}. \tag{4.15}$$

Equipped with these expressions we will now turn to first applications.

4.2 Hamiltonians of identical particles

4.2.1 Hamiltons in second quantization

Being prepared in this fashion, we can describe interacting bosonic systems consisting of N constituents. The single particle state vectors will be denoted as $\{|\psi_k\rangle\}$ with wave function ψ_k. The Hamilton operator can then be written as

$$H^{(N)} = H_0^{(N)} + H_1^{(N)}, \tag{4.16}$$

$$H_0^{(N)} = \sum_{j=1}^{N} F_j, \tag{4.17}$$

$$H_1^{(N)} = \sum_{k>j=1}^{N} V_{j,k}. \tag{4.18}$$

Here F is a single particle operator, V a two particle operator. F_j only acts on the particle labeled j, while $V_{j,k}$ captures the interaction between particles labeled j and k. In matrix form, for each of the F_j, we have

$$F = \sum_{k,l} \langle\psi_l|F|\psi_k\rangle|\psi_l\rangle\langle\psi_k|. \tag{4.19}$$

The matrix with elements

$$\{\langle\psi_l|F|\psi_k\rangle : k, l = 0, 1, \dots\}, \tag{4.20}$$

to state this again, is the matrix that expresses the single particle Hamiltonian F in the single particle state vectors $\{|\psi_k\rangle\}$. We will now try to write this Hamiltonian in terms of creation and annihilation operators. As anticipated, field operators will come to our rescue.

We will see that this Hamiltonian is the projection of

$$\begin{aligned} H &= H_0 + H_1 \\ &= \sum_{j,k} \langle \psi_j | F | \psi_k \rangle b_j^\dagger b_k \\ &+ \frac{1}{4} \sum_{i,j,k,l} \Big(\langle \psi_j, \psi_i | V | \psi_k, \psi_l \rangle + \langle \psi_i, \psi_j | V | \psi_k, \psi_l \rangle \Big) b_j^\dagger b_i^\dagger b_l b_k \end{aligned} \quad (4.21)$$

onto the completely symmetric subspace of the N-particle Hilbert space. The interaction V is local, in that the position representation of the operator V satisfies des Operators V

$$\langle \xi_1', \xi_2' | V | \xi_1, \xi_2 \rangle = V(\xi_1, \xi_2) \delta(\xi_1' - \xi_1) \delta(\xi_2' - \xi_2). \quad (4.22)$$

This is a very natural property of a point interaction. Of course, this interaction is symmetric, in that $V(\xi_1, \xi_2) = V(\xi_2, \xi_1)$. This means that in the position representation, we have

$$\begin{aligned} (\langle \psi_j, \psi_i | V | \psi_k, \psi_l \rangle + \langle \psi_i, \psi_j | V | \psi_k, \psi_l \rangle) &= \int d\xi_1 d\xi_2 \psi_j^*(\xi_1) \psi_i(\xi_2) V(\xi_1, \xi_2) \psi_k(\xi_1) \psi_l(\xi_2) \\ &+ \int d\xi_1 d\xi_2 \psi_j^*(\xi_2) \psi_i(\xi_1) V(\xi_1, \xi_2) \psi_k(\psi_1) \psi_l(\xi_2). \end{aligned} \quad (4.23)$$

From this, it should be clear how to proceed to the interaction term H_1, however. In order to show that the two formulations of the Hamiltonian give rise to the same expressions, we start from H_0. Admittedly, we leave it at that. It should be clear from this argument how to treat H_1 as well, which follows exactly the same logic. We will more precisely show that the two expressions are the same when being computated for arbitrary state vectors. For two arbitrary completely symmetric state vectors $|\psi_N\rangle$ and $|\psi_N'\rangle$ we find

$$\begin{aligned} \langle \psi_N' | H_0 | \psi_N \rangle &= \sum_{j,k} \langle \psi_j | F | \psi_k \rangle \langle \psi_N' | b_j^\dagger b_k | \psi_N \rangle \\ &= \sum_{j,k} \langle \psi_j | F | \psi_k \rangle \langle b_j \psi_N' | b_k \psi_N \rangle, \end{aligned} \quad (4.24)$$

where we merely have moved an annihilation operator into the dual vector. From the defining expressions of bosonic field operators, we find

$$b_j = \int d\xi \psi_j^*(\xi) \Psi(\xi), \quad (4.25)$$

and hence

$$\langle \psi_N' | H_0 | \psi_N \rangle = \sum_{j,k} \int d\xi d\xi' \psi_j^*(\xi') \psi_k(\xi) \langle \psi_j | F | \psi_k \rangle \langle \Psi(\xi') \psi_N | \Psi(\xi) \psi_N \rangle. \quad (4.26)$$

Now we can apply the rule Gl. (4.9) that we have established above. In this way, we get the somewhat tedious expression

$$\begin{aligned}\langle\psi'_N|H_0|\psi_N\rangle &= N\sum_{j,k}\int d\xi d\xi'\psi_j^*(\xi')\psi_k(\xi)\\ &\times \langle\psi_j|F|\psi_k\rangle d\xi_1\dots d\xi_{N-1}d\xi'_1\dots d\xi'_{N-1}\\ &\times (\psi'_N)^*(\xi'_1,\dots,\xi'_{N-1},\xi')\psi_N(\xi_1,\dots,\xi_{N-1},\xi)\\ &\times \langle\o|\Psi(\xi'_1)\dots\Psi(\xi'_{N-1})\Psi^\dagger(\xi_{N-1})\dots\Psi^\dagger(\xi_1)|\o\rangle. \quad (4.27)\end{aligned}$$

Of course, and fortunately, most terms will disappear, as they act onto the vacuum. And so we get

$$\begin{aligned}\langle\psi'_N|H_0|\psi_N\rangle &= N\sum_{j,k}\int d\xi d\xi'\psi_j^*(\xi')\psi_k(\xi)\langle\psi_j|F|\psi_k\rangle d\xi_1\dots d\xi_{N-1}\\ &\times (\psi'_N)^*(\xi_1,\dots,\xi_{N-1},\xi')\psi_N(\xi_1,\dots,\xi_{N-1},\xi). \quad (4.28)\end{aligned}$$

Since the wave functions ψ_N and ψ'_N are symmetric in their arguments, we obtain finally

$$\begin{aligned}\langle\psi'_N|H_0|\psi_N\rangle &= \sum_{l=1}^{N}\sum_{j,k} d\xi_1\dots d\xi_l\dots d\xi_N d\xi'_l \quad (4.29)\\ &\times \psi_j^*(\xi')\psi_k^*(\xi)\langle\psi_j|F|\psi_k\rangle\\ &\times (\psi'_N)^*(\xi_1,\dots,\xi'_l,\dots,\xi_N)\psi_N(\xi_1,\dots,\xi_l,\dots,\xi_N).\end{aligned}$$

This is what we intended to show. Let us remind ourselves that each term is

$$F=\sum_{j,k}\langle\psi_j|F|\psi_k\rangle|\psi_j\rangle\langle\psi_k| \quad (4.30)$$

so that indeed,

$$\langle\psi'_N|H_0|\psi_N\rangle=\langle\psi'_N|\sum_j F_j|\psi_N\rangle. \quad (4.31)$$

We have therefore shown that a Hamilton operator that is composed of single particle terms can equally well be written in terms of creation and annihilation operators. This is done in a way so that the coefficient matrix is nothing but the matrix form of the single body problem. A very similar argument applies to the interacting term H_1, again that the two formulations are identical on the symmetric subspace. It should be obvious that the specifics of F and V do not matter here. We have learned something very important here.

- One can write quantum many-body Hamiltonians in second quantization directly in terms of bosonic creation and annihilation operators. In order to compute Hamiltonians, one does not go back to first quantization and compute expressions in the original Hilbert space. Instead, one can directly remain in the occupation number basis. The coefficients in the Hamiltonian are obtained by solving a one-body and two-body problem once and for all. This is an immense simplification!

- This expression makes sense even if the particle number is not held constant.

Of course, we still have the freedom to pick the state vectors $\{|\psi_j\rangle\}$. One usually picks the energy eigenvectors of the single-particle Hamiltonian F with energy values E_j. This means that the single-particle Hamiltonian then becomes diagonal as

$$F = \sum_l \langle\psi_l|F|\psi_l\rangle|\psi_l\rangle\langle\psi_l| = \sum_l E_l|\psi_l\rangle\langle\psi_l|. \tag{4.32}$$

In the literature, these expressions are often written as

$$\{|\psi_k\rangle : k = 0, 1, \dots\} = \{|k\rangle : k = 0, 1, \dots\}. \tag{4.33}$$

We will, unless there is the risk of confusion, often write the single-particle basis as $\{|k\rangle\}$, even if they are not the eigenvectors of the harmonic oscillator, but some arbitrary single-particle Hamiltonian. In this notation,

$$F = \sum_l E_l|l\rangle\langle l|. \tag{4.34}$$

The resulting expression is so important that it deserves a box in its own right.

General Hamiltonian of bosonic identical particles in second quantization: A general Hamiltonian with two-body interaction takes the form

$$\begin{aligned} H &= H_0 + H_1 \qquad (4.35)\\ &= \sum_j E_j b_j^\dagger b_j + \frac{1}{4}\sum_{i,j,k,l}\left(\langle i,j|V|k,l\rangle + \langle j,i|V|k,l\rangle\right) b_j^\dagger b_i^\dagger b_l b_k. \end{aligned}$$

an.

This Hamiltonian has a simple interpretation. One can interpret the bosonic operators as taking out bosons, letting them interact and putting them back again. The amplitude by which this happens is defined by the single- and two-particle problem. Specifically for the interaction term, one takes out two bosons, lets them interact and places them back. This is a very compact and simple form to capture interacting quantum many-body problems. Again, to derive this form, one only has to solve the one- and two-body problems once and for all, to get the appropriate coefficients. Once this is done, one does not have to return to the microscopic interactions any more. We can hence always think in terms of occupation numbers.

4.2.2 Hamiltonians expressed in field operators

This Hamiltonian is call, as often eluded to already, a *Hamiltonian in second quantization*. The field operators Ψ and $\Psi^\dagger$ are often regarded as "second quantized instances of a wave function". This does not mean that we now have formulated a new quantum mechanics of any sort, or a refinement of the "old" quantum mechanics we are more familiar with: It is still the same quantum theory. It is just a neat, concise, and simple formalism of capturing quantum many-body systems of identical particles. There is some substance, however, to the claim of performing a "second quantization" of wave functions, and we will hint at that in this subsection.

Let us look into that. We focus on the situation of bosonic identical particles in an external potential V_1, interacting via a two-body interaction. In this situation, we have, to start with,

$$F = \frac{P^2}{2M} + V_1, \tag{4.36}$$

which leads for an arbitrary basis set $\{|\psi_k\rangle\}$, using

$$H_0 = \sum_{j,k} \langle \psi_j | F | \psi_k \rangle b_j^\dagger b_k,$$

to the expression

$$H_0 = \int d\xi \sum_j \psi_j^*(\xi) \left(\frac{\hbar^2 \Delta}{2M} + V_1(\xi) \right) \psi_k(\xi) b_j^\dagger b_k. \tag{4.37}$$

Turning to a picture of field operators, this becomes

$$H_0 = \int d\xi \Psi^\dagger(\xi) \left(-\frac{\hbar^2 \Delta}{2M} + V_1(\xi) \right) \Psi(\xi). \tag{4.38}$$

Performing an analogous step for the interacting part of the Hamiltonian, we get the form of a Hamiltonian of particles in a potential in second quantization, expressed in field operators as follows.

Hamiltonians in terms of field operators:

$$\begin{aligned} H &= \int d\xi \Psi^\dagger(\xi) \left(-\frac{\hbar^2 \Delta}{2M} + V_1(\xi) \right) \Psi(\xi) \\ &+ \frac{1}{2} \int d\xi d\xi' \Psi^\dagger(\xi') \Psi^\dagger(\xi) V_2(\xi, \xi') \Psi(\xi) \Psi(\xi'). \end{aligned} \tag{4.39}$$

The first term looks a bit like a single-body operators, despite the fact that it is of course an expression involving field operators. According to the definition of field operators, it is to be read as

$$\Delta \Psi(\xi) = \sum_j b_j \Delta(\psi_j(\xi)). \tag{4.40}$$

The factor $1/2$ originates from the indistinguishability of the configurations ξ, ξ' and ξ', ξ. The total particle number operator expressed in field operators is

$$\int d\xi \Psi^\dagger(\xi) \Psi(\xi), \tag{4.41}$$

the expectation value of which provides the total particle number. In a system consisting of exactly N particles, one has

$$\int d\xi \langle \psi_N | \Psi^\dagger(\xi)\Psi(\xi) | \psi_N \rangle = N. \tag{4.42}$$

Let us be aware of the fact, however, that we can also allow for superpositions of particle numbers, unless a super-selection rule prevents us from doing so. Hence, this particle number can in principle be an arbitrary non-negative real number. It looks like the particle density of a single-particle problem. But again, now Ψ is an operator and not a complex values function.

The analogy to the "first quantization" becomes even more transparent when considering the time evolution of field operators in the Heisenberg picture. This may at first look a bit awkward, but let us not forget that any operator, including a field operator, follows some time evolution in the Heisenberg picture. We have

$$\Psi(\xi, t) = e^{iHt}\Psi(\xi, 0)e^{-iHt} \tag{4.43}$$

for the Hamiltonian (4.39), again setting $/\hbar = 1$. Writing this in differential form, we get the differential equation

$$\begin{aligned} i\hbar\frac{\partial}{\partial t}\Psi(\xi, t) &= \left(-\frac{\hbar^2\Delta}{2M} + V_1(\xi)\right)\Psi(\xi, t) \\ &+ \int d\xi' \Psi^\dagger(\xi', t)V_2(\xi, \xi')\Psi(\xi', t)\Psi(\xi, t). \end{aligned} \tag{4.44}$$

This is an equation of motion taking the form of a non-linear Schrödinger equation, or even a linear Schrödinger equation in the simple case of having no interaction whatseoever. This is quickly shown. One starts from the Heisenberg equations of motion

$$\begin{aligned} i\frac{\partial}{\partial t}\Psi(\xi, t) &= -[H, \Psi(\xi, t)] \\ &= -e^{iHt}[H, \Psi(\xi, 0)]e^{-iHt}, \end{aligned} \tag{4.45}$$

and makes use of the general property of commutators

$$[AB, C] = A[B, C] + [A, C]B. \tag{4.46}$$

Again, we see the formal resemblance with the single-body picture of basic quantum mechanics.