Chapter 4

Second quantisation

We now want to introduce the formalism of second quantisation, which provides a way to deal with systems involving multiple particles.

4.1 Two particles

We start by considering systems with two particles. A possible Hamiltonian for a two-particle system is

$$\hat{H} = \frac{\hat{\boldsymbol{p}}_1^2}{2m} + U(\boldsymbol{r}_1) + \frac{\hat{\boldsymbol{p}}_2^2}{2m} + U(\boldsymbol{r}_2) + U_{\text{int}}(\boldsymbol{r}_1, \boldsymbol{r}_2).$$

Here $\boldsymbol{r}_1$ and $\boldsymbol{r}_2$ are the positions of the two particles, $\hat{\boldsymbol{p}}_1$ and $\hat{\boldsymbol{p}}_2$ are the corresponding momentum operators, m is the mass (assumed to be the same for both particles) and U is the potential (also assumed to be the same). In addition there is a potential term $U_{\text{int}}(\boldsymbol{r}_1, \boldsymbol{r}_2)$ that depends on the positions of both particles and describes their interaction. For example, electric attraction/repulsion or gravitational attraction leads to $U_{\text{int}}(\boldsymbol{r}_1, \boldsymbol{r}_2) = \frac{a}{|\boldsymbol{r}_1 - \boldsymbol{r}_2|}$ with suitably chosen a.

Hilbert space. The Hilbert space of the two-particle system is the space of all possible wavefunctions $\psi(\boldsymbol{r}_1, \boldsymbol{r}_2)$ depending on both positions. As usual these wavefunctions are assumed to be square integrable.

Basis. Now assume that we are using a **basis** $\psi_i(\boldsymbol{r})$ for the Hilbert space of single-particle wavefunctions. (E.g. these could be eigenfunctions of the single particle Hamiltonian $\frac{\hat{\boldsymbol{p}}^2}{2m} + U(\boldsymbol{r})$ but we could also use any other basis.) In Dirac notation these basis functions will be written as $|i\rangle$. Then a suitable basis for the Hilbert space of two-particle wavefunctions is provided by the products of single-particle basis functions $\psi_i(\boldsymbol{r}_1)\psi_j(\boldsymbol{r}_2)$. In Dirac notation these basis functions are indicated by the tensor products $|i\rangle \otimes |j\rangle$, or if one omits the tensor product sign one simply writes $|i\rangle|j\rangle$.

Indistinguishable particles. Importantly, quantum mechanical particles of the same type (such as electrons, protons, etc) are indistinguishable from each other. This means that for a system of, say, two such particles the result of a measurement might indicate that one particle is at position $\boldsymbol{r}_1$ and the other particle is at position $\boldsymbol{r}_2$. However as the particles are indistinguishable we can't tell apart the case that the first particle is at $\boldsymbol{r}_1$ and the second one is at $\boldsymbol{r}_2$ and the case that the first one is at $\boldsymbol{r}_2$ and the second one is at $\boldsymbol{r}_1$.

This has important consequences for the corresponding wavefunctions. The probability density for finding the first particle at $\boldsymbol{r}_1$ and the second particle at $\boldsymbol{r}_2$ is given by $|\psi(\boldsymbol{r}_1, \boldsymbol{r}_2)|^2$ whereas the probability density for finding the first particle at $\boldsymbol{r}_2$ and the second particle at $\boldsymbol{r}_1$ is $|\psi(\boldsymbol{r}_2, \boldsymbol{r}_1)|^2$. If both events are indistinguishable we must have

$$|\psi(\boldsymbol{r}_2, \boldsymbol{r}_1)|^2 = |\psi(\boldsymbol{r}_1, \boldsymbol{r}_2)|^2$$

and hence

$$\psi(\boldsymbol{r}_2, \boldsymbol{r}_1) = e^{i\phi}\psi(\boldsymbol{r}_1, \boldsymbol{r}_2).$$

It turns out (this is a law of nature) that the choice of $e^{i\phi}$ depends on the type of particle:

- For **bosons** (e.g. photons - the particles associated with light) we always have $e^{i\phi} = 1$.
- For **fermions** (e.g. electrons, protons,...) we always have $e^{i\phi} = -1$.
- Other choices of $e^{i\phi}$ are not possible for fundamental particles.

Particles composed of these building blocks, e.g., atoms or molecules may be bosons or fermions. It turns out that more elaborate ways of building 'effective' particles from fundamental building blocks even allow for particles with other $e^{i\phi}$, so-called anyons.

Spin. Quantum mechanical particles appearing in nature also often have spin. In spin systems the wavefunction assumes a vector form with components $\psi_\sigma(\boldsymbol{r})$. Equivalently we could regard the index σ as part of the argument and write $\psi(\sigma, \boldsymbol{r})$ if we remember that σ has to be discrete. For systems with spin everything said here carries over if we replace $\boldsymbol{r}$ by $(\sigma, \boldsymbol{r})$. Writing $\boldsymbol{r}$ only is just a convenient way to simplify notation.

If one goes deeper in the theory of spin one realises that for bosons the number of spin components must be odd (this includes the case of single component wavefunctions and hence no spin) whereas for fermions it must be even.

Hilbert space. The Hilbert space for systems of two bosons is the space of (square-integrable) wavefunctions $\psi(\boldsymbol{r}_1, \boldsymbol{r}_2)$ satisfying $\psi(\boldsymbol{r}_2, \boldsymbol{r}_1) = \psi(\boldsymbol{r}_1, \boldsymbol{r}_2)$. For fermions the condition is replaced by $\psi(\boldsymbol{r}_2, \boldsymbol{r}_1) = -\psi(\boldsymbol{r}_1, \boldsymbol{r}_2)$

Basis. The basis functions of this new Hilbert space also have to be (anti-)symmetric with respect to particle exchange. Using the basis of single particle wavefunctions $\psi_i(\boldsymbol{r})$ (anti-) symmetric functions can be constructed as follows:

$$\psi_{ij}(\boldsymbol{r}_1, \boldsymbol{r}_2) = C(\psi_i(\boldsymbol{r}_1)\psi_j(\boldsymbol{r}_2) \pm \psi_j(\boldsymbol{r}_1)\psi_i(\boldsymbol{r}_2)). \tag{4.1}$$

Here the plus sign is for bosons and the minus sign for fermions, and C is a normalisation constant to be determined later. $\psi_{ij}(\boldsymbol{r}_1, \boldsymbol{r}_2)$ is the *only* bosonic/fermionic state with one particle in the single-particle state i and one article in the single particle state j. This contrasts with the case of distinguishable particles where we have (for $i \neq j$) two basis functions with one particle in state i and one in state j, namely $\psi_i(\boldsymbol{r}_1)\psi_j(\boldsymbol{r}_2)$ and $\psi_j(\boldsymbol{r}_1)\psi_i(\boldsymbol{r}_2)$. In Dirac notation our bosonic/fermionic basis states can be written as

$$|i, j\rangle = C(|i\rangle|j\rangle \pm |j\rangle|i\rangle).$$

Pauli exclusion principle. Importantly, for fermions we have $\psi_{ii}(\boldsymbol{r}_1, \boldsymbol{r}_2) = 0$, i.e., there is no basis state where both particles are in the single-particle state i. The inability of fermions to be both in the same state is known as Pauli's exclusion principle. (Note that if spin is taken into account, this means that the two particles cannot be in the same state as characterised by position *and* spin!)

Normalisation. We still have to determine C. We demand our single-particle states to be normalised and orthogonal to each other, i.e.,

$$\int d^n r\, \psi_i^*(\boldsymbol{r})\psi_{i'}(\boldsymbol{r}) = \delta_{ii'}.$$

Then the same applies to the two-particle states $\psi_i(\boldsymbol{r}_1)\psi_j(\boldsymbol{r}_2)$ where indistinguishability is not yet taken into account,

$$\begin{aligned} & \int d^n r_1 \int d^n r_2\, (\psi_i(\boldsymbol{r}_1)\psi_j(\boldsymbol{r}_2))^*(\psi_{i'}(\boldsymbol{r}_1)\psi_{j'}(\boldsymbol{r}_2)) \\ = & \left(\int d^n r_1 \psi_i(\boldsymbol{r}_1)^*\psi_{i'}(\boldsymbol{r}_1)\right)\left(\int d^n r_2 \psi_j(\boldsymbol{r}_2)^*\psi_{j'}(\boldsymbol{r}_2)\right) \\ = & \delta_{ii'}\delta_{jj'} \end{aligned} \tag{4.2}$$

We now want to choose C such that the $\psi_{ij}(\boldsymbol{r}_1, \boldsymbol{r}_2)$ defined in (4.1) satisfies

$$1 = \int d^n r_1 d^n r_2 |\psi_{ij}(\boldsymbol{r}_1, \boldsymbol{r}_2)|^2.$$

We first consider $i \neq j$, and assume that C is positive. If we insert (4.1) we then get C^2 times the norm of $\psi_i(\boldsymbol{r}_1)\psi_j(\boldsymbol{r}_2)$ which is 1, C^2 times the norm of $\psi_j(\boldsymbol{r}_1)\psi_i(\boldsymbol{r}_2)$ which is also 1, C^2 times scalar products of $\psi_i(\boldsymbol{r}_1)\psi_j(\boldsymbol{r}_2)$ and $\psi_j(\boldsymbol{r}_1)\psi_i(\boldsymbol{r}_2)$ which are zero. Hence we have

$$1 = C^2(1 + 1) \Rightarrow C = \frac{1}{\sqrt{2}}.$$

For bosonic states with two particles occupying the single particle state i we have

$$\psi_{ii}(\boldsymbol{r}_1, \boldsymbol{r}_2) = \psi_i(\boldsymbol{r}_1)\psi_i(\boldsymbol{r}_2)$$

which is normalised due to (4.2).

4.2 N particles

Hilbert space. For N-particle systems the wavefunction can be written as $\psi(\boldsymbol{r}_1, \boldsymbol{r}_2, \ldots, \boldsymbol{r}_N)$. The conditions on ψ are analogous to the case of two particles. For bosons the wavefunction has to be symmetric w.r.t. exchanges of any two of the arguments, and for fermions it has to be antisymmetric w.r.t. such exchanges.

Basis. We want to build basis states similar to the case of two particles, first for **bosons**. Let $\psi_{i_1,\ldots,i_N}(\boldsymbol{r}_1, \ldots, \boldsymbol{r}_N)$ be the many particle state in which the single-particle states $i_1, \ldots, i_N$ are occupied. (For bosons some or all of the states may coincide.) One might at first consider the product state $\psi_{i_1}(\boldsymbol{r}_1) \ldots \psi_{i_N}(\boldsymbol{r}_N)$. However this is not symmetric w.r.t. exchanging arguments so in analogy to the case of two particles we symmetrise and consider

$$\begin{aligned} & \psi_{i_1,\ldots,i_N}(\boldsymbol{r}_1, \ldots, \boldsymbol{r}_N) \\ = \; & C(\psi_{i_1}(\boldsymbol{r}_1) \ldots \psi_{i_N}(\boldsymbol{r}_N) + \text{all terms where indices are interchanged}). \end{aligned}$$

Here one could exchange either the indices of the ψ's or the indices of the $\boldsymbol{r}$'s but the usual convention is to exchange the former.

For **fermions** any exchange of two particles should flip the sign. Hence for the terms with exchanged indices we imagine the exchanges to be performed in steps, and in each step just two indices are interchanged. If the number of these steps (transpositions) is even the sign flips compensate. For the terms involving an odd number of transpositions there is an overall minus sign.

Permutations. To formalise these results mathematically we need permutations:

- A permutation of the integers $1, 2, \ldots, N$ is defined as a bijective mapping between these numbers. As a consequence of the mapping being bijective no two numbers may be mapped to the same number.
- One can show that every permutation may be obtained by successive application of transpositions. These are permutations in which just two numbers interchanged, and all other numbers are mapped to themselves.
- A given permutation can be written in terms of different numbers of transpositions. (E.g. one could always add another transposition that interchanges two numbers, and a further transposition that undoes this exchange.) However one can show for a given permutation the number of transpositions is always odd or even. Hence it makes sense to define the sign of a permutation π as

$$\operatorname{sign} \pi = \begin{cases} +1 & \text{if the number of transpositions is even} \\ -1 & \text{if the number of transpositions is odd.} \end{cases}$$

With permutations the basis functions introduced above can be written as

$$\psi_{i_1,\ldots,i_N}(\boldsymbol{r}_1,\ldots,\boldsymbol{r}_N) = C\sum_{\pi}\psi_{i_{\pi(1)}}\ldots\psi_{i_{\pi(N)}}(\boldsymbol{r}_1,\ldots,\boldsymbol{r}_N)\times\begin{cases}1 & \text{for bosons}\\ \operatorname{sign}\pi & \text{for fermions.}\end{cases}$$

We note that using the representation of the determinant in terms of a sum over permutations the result for the fermionic case can be written as a determinant (the so called Slater determinant).

Normalisation. Similarly as for two-particle states we have to choose C such that the basis functions are normalised. If one works this out (this will be done on a problem sheet for the case $N = 3$) one obtains for fermions

$$C = \frac{1}{\sqrt{N!}}.$$

For bosons we also have to take into account the possibility that there are several particles in the same state. Then one obtains

$$C = \frac{1}{\sqrt{N!\prod_i n_i!}}$$

where n_i is the number of particles in state i.

4.3 Fock space

In quantum mechanics we can have the situation that we don't know how many particles there are in our system. The number of particles is an observable (measurable quantity) like positions and momenta. If we have not performed a measurement of the particle number (or set the system up to have a given number of particles from the start) the number of particles may be unknown similar to a position or momentum being unknown if we have not made a corresponding measurement. States where the number of particles is not fixed can be written as **quantum superpositions of states with different numbers of particles**.

In this superposition we even have to allow for the possibility of having no particles at all. The quantum state with no particles at all is called the **vacuum**. In Dirac notation the vacuum is denoted by $|0\rangle$. We stress that this is a valid quantum mechanical state and it has to be distinguished from zero.

If we denote by $\mathcal{F}_N$ the Hilbert space of (bosonic or fermionic) N particle wavefunctions, the Hilbert space of all permissible states (the **Fock space**) is formed by linear combinations of elements of all $\mathcal{F}^N$. The space of all linear combinations of elements of a number of vector spaces is called the direct sum of these vector spaces. Hence the Fock space can be formally defined as

$$\mathcal{F} = \bigoplus_{N=0}^{\infty}\mathcal{F}_N$$

where $\bigoplus$ indicates a direct sum.

Note: If we have a linear combination of states with different N its component for each N can be written as a wavefunction with N arguments. But the linear combination as a whole cannot be written as a wavefunction with a well-defined number of parameters.

4.4 Creation and annihilation operators

Occupation number representation. In order to do calculations in Fock space it is helpful to use creation and annihilation operators. To define these operators we represent our states in occupation number representation. In this representation the multiple-particle basis states are indicated by $|n_1, n_2, \ldots\rangle$ where n_i indicates the number of particles that are in the single particle state i. Translated into the notation used earlier we thus have

$$|n_1, n_2, \ldots\rangle = |\underbrace{1, \ldots, 1}_{n_1 \text{ entries}}, \underbrace{2, \ldots, 2}_{n_2 \text{ entries}}, \ldots\rangle.$$

The occupation number representation can also be used for fermions; in this case all n_i are either 0 or 1. The bra associated to $|n_1, n_2, \ldots\rangle$ is written as

$$\langle n_1, n_2, \ldots|.$$

Creation and annihilation operators for bosons. The creation operator $a_i^\dagger$ is defined such that it increases the number of particles in state i by 1 and multiplies the state with a factor $\sqrt{n_i + 1}$:

$$a_i^\dagger |n_1, \ldots, n_i, \ldots\rangle = \sqrt{n_i + 1}|n_1, \ldots, n_i + 1, \ldots\rangle. \tag{4.3}$$

The annihilation operator a_i removes a particle in state i and multiplies with $\sqrt{n_i}$:

$$a_i |n_1, \ldots, n_i, \ldots\rangle = \sqrt{n_i}|n_1, \ldots, n_i - 1, \ldots\rangle. \tag{4.4}$$

If the annihilation operator a_i is applied to a state with $n_i = 0$ the prefactor makes sure that the resulting state is identically zero. This is needed for consistency as we can't have a multiple-particle states with -1 particles in state i.

Note that we are not free to choose the prefactors in these definitions as we like. For example we would like a_i and $a_i^\dagger$ to be adjoints of each other, and we want the above behaviour in case of $n_i = 0$. The arising factors are analogous to the raising and lowering operators in the algebraic approach to the harmonic oscillator. However we will not dwell further on the precise constraints for choosing the prefactors in the present case.

Commutators. The commutators $[A, B] = AB - BA$ of the creation and annihilation operators are

$$[a_i, a_j] = 0, \qquad [a_i^\dagger, a_j^\dagger] = 0, \qquad [a_i, a_j^\dagger] = \delta_{ij}. \tag{4.5}$$

Proof: Each creation and annihilation operator just modifies the occupation number corresponding to its index, and multiplies with a factor only depending on this number. Hence the ordering or creation and annihilation operators with different indices does not matter, and all operators with $i \neq j$ commute.

For $i = j$ we trivially have $[a_i, a_i] = 0$ and $[a_i^\dagger, a_i^\dagger] = 0$. The only nontrivial commutator is $[a_i, a_i^\dagger]$. If we apply this commutator to a state $|\ldots, n_i, \ldots\rangle$ we obtain

$$\begin{aligned}
& [a_i, a_i^\dagger]|\ldots, n_i, \ldots\rangle \\
= \;& a_i a_i^\dagger |\ldots, n_i, \ldots\rangle - a_i^\dagger a_i |\ldots, n_i, \ldots\rangle \\
= \;& a_i \sqrt{n_i + 1} |\ldots, n_i + 1, \ldots\rangle - a_i^\dagger \sqrt{n_i} |\ldots, n_i - 1, \ldots\rangle \\
= \;& (n_i + 1)|\ldots, n_i, \ldots\rangle - n_i |\ldots, n_i, \ldots\rangle \\
= \;& |\ldots, n_i, \ldots\rangle
\end{aligned} \tag{4.6}$$

Here we used only the definitions (4.3) and (4.4). Note that in the next-to-last line we applied a_i to a state where the occupation number n_i is replaced by $n_i + 1$, hence the factor $\sqrt{n_i}$ in (4.4) is replaced by $\sqrt{n_i + 1}$ which has to be multiplied with the $\sqrt{n_i + 1}$ already there; the second term in that line is obtained similarly. As $[a_i, a_i^\dagger]$ acts like 1 on all basis states, it has to act like 1 on all states of the Fock space.

Particle number operator. If we consider the second terms in all lines of (4.6) we see that

$$a_i^\dagger a_i |\ldots, n_i, \ldots\rangle = n_i |\ldots, n_i, \ldots\rangle$$

i.e. $a_i^\dagger a_i$ is the operator giving the number of particles in state i.

4.5 Hamiltonian in second quantisation

We now want to write down the Hamiltonian of a multiple-particle quantum system in second quantisation, using creation and annihilation operators.

Example. We start by considering an example system where the particles can only be on discrete sites, labelled by $1, 2, 3, \ldots$. For this system the single-particle wavefunctions are just vectors

$$\begin{pmatrix} \psi(1) \\ \psi(2) \\ \vdots \end{pmatrix}$$

The single-particle Hamiltonian is chosen to mimick

$$\hat{H}\psi(x) = \left(-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + U(x) \right) \psi(x).$$

The discrete analogue of the second derivative of $\psi(x)$ is[1]

$$\psi(x+1) - 2\psi(x) + \psi(x-1)$$

Hence for the discrete system we have

$$(\hat{H}\psi)(x) = -\frac{\hbar^2}{2m}(\psi(x+1) - 2\psi(x) + \psi(x-1)) + U(x)\psi(x). \tag{4.7}$$

In matrix form the Hamiltonian thus becomes

$$\hat{H} = -\frac{\hbar^2}{2m}\begin{pmatrix} -2 & 1 & & \\ 1 & -2 & 1 & \\ & 1 & -2 & \ddots \\ & & \ddots & \ddots \end{pmatrix} + \begin{pmatrix} U(1) & & & \\ & U(2) & & \\ & & U(3) & \\ & & & \ddots \end{pmatrix} \tag{4.8}$$

Multi-particle Hamiltonian. Now let us consider a system with discrete sites, but allow for multiple particles. Then the corresponding Hamiltonian will act on wavefunctions $\psi(x_1, x_2, \ldots, x_N)$. It is given by

$$\hat{H}_{\text{mult}} = \sum_{p=1}^{N} \hat{H}_p + \frac{1}{2} \sum_{\substack{p,p'=1,\ldots,N \\ p \neq p'}} U_{\text{int}}(x_p, x'_p). \tag{4.9}$$

Here the part $\hat{H}_p$ gives the energy of the p-th particle. It is defined as in (4.7) w.r.t. the variable x_p taking the role of x. In addition different particles can interact. For example an electric or gravitational interaction between the particles p and p' would lead to an interaction potential of the form $\frac{a}{|x_p - x_{p'}|}$. In general the potential due to interaction of particles at x_p and $x_{p'}$ is denoted by $U_{\text{int}}(x_p, x_{p'})$. This needs to be summed over all particles p and p'. However, in the sum we have to exclude the terms $p = p'$ as a particle does not interact with itself. (For example, a particle does not gravitationally attract or electrically repel itself.) Moreover, if we let the sums over p and p' run over all particles the interaction between two particles will formally be counted twice as we could choose the first particle as p and the second one as p' or the other way around. To compensate this we have divided by 2 in (4.9).

Second quantisation. We now want to write $\hat{H}_{\text{mult}}$ in the formalism of second quantisation, using creation and annihilation operators $a_i^\dagger$, a_i. To do so we have to choose a basis of single particle wavefunctions $\psi_i(x)$. We simply take the wavefunctions localised at the site i, i.e. $\psi_i(x) = \delta_{xi}$. (Note that here x is a discrete argument.)

We have to consider all terms present in (4.8) and (4.9):

[1] To show this, note that the first derivative is given by $\psi'(x) = \lim_{\Delta x \to 0} \frac{\psi(x+\Delta) - \psi(x)}{\Delta x}$. In the discrete case we can't take Δx to zero, the best thing we can do is take Δx to 1. This gives $\psi(x+1) - \psi(x)$ as the analogue of the first derivative, but we could also take $\psi(x) - \psi(x-1)$. If we take $f(x) = \psi(x+1) - \psi(x)$ as the counterpart of the first derivative and $g(x) = f(x) - f(x-1)$ as the counterpart of the second derivative we get

$$g(x) = f(x) - f(x-1) = (\psi(x+1) - \psi(x)) - (\psi(x) - \psi(x-1)) = \psi(x+1) - 2\psi(x) + \psi(x-1)$$

as used above.

- **Potential:** Each particle at site i feels the potential $U(i)$, and the number of all particles at site i can be obtained by applying the particle number operator $a_i^\dagger a_i$. Hence the total potential is obtained by applying the operator

$$\sum_i U(i) a_i^\dagger a_i. \tag{4.10}$$

- **Single particle Hamiltonian:** For the total contribution of the single particle Hamiltonians we will only make an educated guess (but one can prove that it's correct). We are guided by the observation that the potential is represented by a diagonal matrix in (4.8), and this gives rise to a sum over the diagonal elements multiplied with $a_i^\dagger a_i$ where i is the index of the corresponding row as well as the corresponding column. By contrast the full single particle Hamiltonian in (4.7) is given by a matrix containing off-diagonal elements. The natural generalisation of the formula (4.10) to the off-diagonal single-particle Hamiltonians as in (4.8) is therefore

$$\sum_{i,j} H(i,j) a_i^\dagger a_j.$$

  Here $H(i,j)$ are the matrix elements.

- **Interactions:** The interaction potential between two particles at sites i, j can be written as $U_{\text{int}}(i,j)$. If $i \neq j$ such a potential arises for all pairs of particles at i and j. To get the number of pairs we multiply the number of particles in state i, obtained using the operator $a_i^\dagger a_i$, with the number of particles in state j, obtained using the operator $a_j^\dagger a_j$. In the case $i = j$ both particles are at the same site, so they could potentially be the same. However we should not include self-interaction. Hence in the case $i = j$ the number of choices for the second particle should be reduced by 1, meaning that in general the number of choices for the second particle is $a_j^\dagger a_j - \delta_{ij}$. The overall interaction potential is therefore given by the operator

$$\frac{1}{2} \sum_{i,j} U_{\text{int}}(i,j) a_i^\dagger a_i (a_j^\dagger a_j - \delta_{ij}).$$

  Here the reasons for the factor $\frac{1}{2}$ are the same as in Eq. (4.9).

  Theorem: The combination of operators above can be simplified as

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

  Proof: We have

$$a_i^\dagger a_j^\dagger a_j a_i = a_i^\dagger a_j^\dagger a_i a_j = a_i^\dagger (a_i a_j^\dagger - \underbrace{(a_i a_j^\dagger - a_j^\dagger a_i)}_{=[a_i, a_j^\dagger] = \delta_{ij}}) a_j = a_i^\dagger a_i a_j^\dagger a_j - \delta_{ij} a_i^\dagger a_j$$

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

  Here we have used in the first step that $[a_j, a_i] = 0$, and in the final step that $\delta_{ij} a_i^\dagger a_j$ only contributes if $i = j$.

With these results the full multiple-particle Hamiltonian can be written as

$$\hat{H}_{\text{mult}} = \sum_{i,j} H(i,j) a_i^\dagger a_j + \frac{1}{2} \sum_{i,j} U_{\text{int}}(i,j) a_i^\dagger a_j^\dagger a_j a_i.$$

Continuous case. We also want to state the result for the case of continuous positions in $\mathbb{R}^n$ instead of discrete sites. In this case the indices i, j are replaced by $\boldsymbol{r}, \boldsymbol{r}' \in \mathbb{R}^n$. The operator $a^\dagger(\boldsymbol{r})$ creates a particle at position $\boldsymbol{r}$. In this case the potential term (4.10) becomes $\int d^n r\, U(\boldsymbol{r}) a^\dagger(\boldsymbol{r}) a(\boldsymbol{r}) = \int d^n r\, a^\dagger(\boldsymbol{r}) U(\boldsymbol{r}) a(\boldsymbol{r})$. The off-diagonal parts in (4.8) were arising from a discretisation of the second derivative in the kinetic energy $-\frac{\hbar^2}{2m}\nabla^2$ (where for $n = 1$, $\nabla = \frac{d}{dx}$). In the continuous case this discretisation is undone and we get back the derivatives, the kinetic energy then becomes $\int d^n r\ a^\dagger(\boldsymbol{r}) \left(-\frac{\hbar^2}{2m}\nabla^2\right) a(\boldsymbol{r})$. In the interaction potential term we simply replace discrete variables by continuous ones and sums by integrals. The overall result is

$$\begin{aligned} \hat{H}_{\text{mult}} &= \int d^n r\ a^\dagger(\boldsymbol{r}) \left(-\frac{\hbar^2}{2m}\nabla^2 + U(\boldsymbol{r})\right) a(\boldsymbol{r}) \\ &+ \frac{1}{2}\int d^n r d^n r' U_{\text{int}}(\boldsymbol{r}, \boldsymbol{r}') a^\dagger(\boldsymbol{r}) a^\dagger(\boldsymbol{r}') a(\boldsymbol{r}') a(\boldsymbol{r}). \end{aligned}$$

Historically this formula is the reason for the term 'second quantisation'. If we replace the operator $a(\boldsymbol{r})$ by the wavefunction $\psi(\boldsymbol{r})$ and $a^\dagger(\boldsymbol{r})$ by $\psi^*(\boldsymbol{r})$ the noninteracting part of the Hamiltonian looks like the expectation value of the energy in the state $\psi(\boldsymbol{r})$,

$$\int d^n r\ \psi^*(\boldsymbol{r}) \left(-\frac{\hbar^2}{2m}\nabla^2 + U(\boldsymbol{r})\right) \psi(\boldsymbol{r}).$$

Hence the noninteracting part looks as we had taken the wavefunction and turned it into a quantum operator, similarly to what is done with positions and momenta in 'first' quantisation. For this reason $a^\dagger(\boldsymbol{r}), a(\boldsymbol{r})$ are often written as $\hat{\psi}^\dagger(\boldsymbol{r}), \hat{\psi}(\boldsymbol{r})$.

4.6 Fermions

So far we have defined creation and annihilation operators only for bosons. For fermions we have to take into account that due to Pauli's exclusion principle the only possible occupation numbers are 0 and 1. However if the creation operator $a_i^\dagger$ is applied twice we would expect it to create two particles in state i and hence lead to a many-particle state violating the exclusion principle. The only way out is to demand $(a_i^\dagger)^2 = 0$. If we introduce the anticommutator of any two operators

$$[A, B]_+ = AB + BA$$

this implies

$$[a_i^\dagger, a_i^\dagger]_+ = 0$$

reminding of the relation $[a_i^\dagger, a_i^\dagger] = 0$ for bosons. Hence a mathematically satisfying definition of creation and annihilation operators for fermions might be one that yields all boson commutation relations (4.5) with commutators replaced by anticommutators:

$$[a_i, a_j]_+ = 0, \qquad [a_i^\dagger, a_j^\dagger]_+ = 0, \qquad [a_i, a_j^\dagger]_+ = \delta_{ij}. \tag{4.11}$$

A definition satisfying these conditions is the following

$$
\begin{aligned}
a_i^\dagger|\ldots n_i = 0\ldots\rangle &= (-1)^{\sum_{k=1}^{i-1} n_k}|\ldots n_i = 1\ldots\rangle && (4.12)\\
a_i^\dagger|\ldots n_i = 1\ldots\rangle &= 0 && (4.13)\\
a_i|\ldots n_i = 0\ldots\rangle &= 0 && (4.14)\\
a_i|\ldots n_i = 1\ldots\rangle &= (-1)^{\sum_{k=1}^{i-1} n_k}|\ldots n_i = 0\ldots\rangle && (4.15)
\end{aligned}
$$

where we have to consider only the cases that each operator acts on a state with $n_i = 0$ or $n_i = 1$.

Motivation

- As expected (4.12) implies that $a_i^\dagger$ creates a particle in state i if it is applied to a many-particle state with $n_i = 0$. Eq (4.15) indicates that the annihilation operator annihilates a particle in state i if there is one to annihilate. The only aspect of these cases still to be understood are the sign factors.

- Eqs. (4.13) and (4.14) are required in order to avoid particle numbers different from 0 and 1. When applied to a state with a particle already present the creation operator may not create a second particle so we obtain 0 instead. The annihilation operator applied to a state without a corresponding particle present returns zero as states with $n_i = -1$ are not permitted.

- The signs in (4.12) and (4.15) are needed in order to satisfy the anticommutation relations. To understand this imagine we wouldn't have these signs. Then we would obtain, in the example of a system with two states,

$$
\begin{aligned}
a_1^\dagger a_2^\dagger|0,0\rangle = a_1^\dagger|0,1\rangle = |1,1\rangle\\
a_2^\dagger a_1^\dagger|0,0\rangle = a_2^\dagger|1,0\rangle = |1,1\rangle.
\end{aligned}
$$

  This contradicts the requirement $a_1^\dagger a_2^\dagger = -a_2^\dagger a_1^\dagger$. However in our example the requirement is satisfied with the sign factors as in this case we have

$$
\begin{aligned}
a_1^\dagger a_2^\dagger|0,0\rangle = a_1^\dagger|0,1\rangle = |1,1\rangle\\
a_2^\dagger a_1^\dagger|0,0\rangle = a_2^\dagger|1,0\rangle = -|1,1\rangle.
\end{aligned}
$$

- Let us now consider general $a_i^\dagger$ and $a_j^\dagger$ with $i < j$, and check that the above definition satifies the correct anticommutation relation. To do so it is sufficient to apply $a_i^\dagger a_j^\dagger$ and $a_j^\dagger a_i^\dagger$ to a general basis state with $n_i = n_j = 0$. Other basis states need not be considered as we know that application of either product will map them to zero. For the basis states under consideration we obtain

$$
\begin{aligned}
& a_i^\dagger a_j^\dagger|\ldots n_i = 0\ldots n_j = 0\ldots\rangle\\
= \; & a_i^\dagger(-1)^{\sum_{k=1}^{j-1} n_k}|\ldots n_i = 0\ldots n_j = 1\ldots\rangle\\
= \; & (-1)^{\sum_{k=1}^{i-1} n_k}(-1)^{\sum_{k=1}^{j-1} n_k}|\ldots n_i = 1\ldots n_j = 1\ldots\rangle
\end{aligned}
$$

and similarly

$$\begin{aligned} & a_j^\dagger a_i^\dagger |\dots n_i = 0 \dots n_j = 0 \dots\rangle \\ = \;& a_j^\dagger (-1)^{\sum_{k=1}^{i-1} n_k} |\dots n_i = 1 \dots n_j = 0 \dots\rangle \\ = \;& (-1)^{\sum_{k=1}^{j-1} n_k + 1} (-1)^{\sum_{k=1}^{i-1} n_k} |\dots n_i = 1 \dots n_j = 1 \dots\rangle. \end{aligned}$$

In the second calculation the important difference is that $a_j^\dagger$ acts on a state where n_i is 1 rather than 0. As the summands n_k in the formula are defined according to the initial basis state the operators were applied to (with $n_i = 0$) we thus have to add 1 to the sum arising from $a_j^\dagger$. As a result the states obtained by applying $a_i^\dagger a_j^\dagger$ and $a_j^\dagger a_i^\dagger$ differ by a sign factor, as desired.

- A full check of the commutation relations as well as the adjointness of a_i and $a_i^\dagger$ is made on a problem sheet.