Chapter 1

Many-body quantum mechanis

1.1 Distinguishable systems and the tensor product

Consider two particles moving in one dimension. The Hilbert space of each particle is $L^2(\mathbb{R})$, the space of wave functions over $\mathbb{R}$. Let $\{|x\rangle\}_{x\in\mathbb{R}}$ be the position basis for one particle.

What is the Hilbert space for the total system, comprising both particles?

There is a natural guess. We could try the Hilbert space with basis

$$|x_1, x_2\rangle, \qquad x_i \in \mathbb{R}. \tag{1.1}$$

This Hilbert space is, in fact, $L^2(\mathbb{R}^2)$, the space of wave functions $\psi(x_1, x_2)$ with two arguments.

This choice makes sense for all kinds of reasons. For example, it means that both in the single and in the two-particle case, we would use the set of wave functions over the classical configuration space as the Hilbert space. Nicely consistent. On $L^2(\mathbb{R}^2)$, we can also define position- and momentum operators

$$X_i\,\psi(x_1, x_2) := x_i\psi(x_1, x_2), \qquad P_i\,\psi(x_1, x_2) := -\mathrm{i}\hbar\partial_{x_i}\psi(x_1, x_2). \tag{1.2}$$

They satisfy the *canonical commutation relations*

$$[X_i, P_j] = \mathrm{i}\hbar\delta_{i,j},$$

which, according to the *canonical quantization* heuristic, is what we should aim for when quantizing classical mechanical systems. The guess (1.1) seems to work well!

Likeweise, given two spin-1/2 systems whose Hilbert spaces are spanned by

$$\{|+\tfrac{1}{2}\rangle, |-\tfrac{1}{2}\rangle\},$$

it is plausible to guess that

$$|+\frac{1}{2},+\frac{1}{2}\rangle, \quad |+\frac{1}{2},-\frac{1}{2}\rangle, \quad |-\frac{1}{2},+\frac{1}{2}\rangle, \quad |-\frac{1}{2},-\frac{1}{2}\rangle \tag{1.3}$$

forms a basis for the total Hilbert space.

These guesses turn out to give the right answer *for some classes of systems* – namely for *distinguishable particles*. Mathematically, the construction is called the *tensor product* of Hilbert spaces. We introduce the tensor product formally below, before we turn to alternative ways for building global Hilbert spaces.

1.1.1 Tensor products

Let $\mathcal{H}_1, \mathcal{H}_2$ be two Hilbert spaces, with respective ONBs $\{|e_i\rangle\}_i, \{|f_j\rangle\}_j$. Their *tensor product* $\mathcal{H}_1 \otimes \mathcal{H}_2$ is the space of linear combinations of the symbols $|e_i\rangle \otimes |f_j\rangle$. As usual, there are various short-hand notations used in physics:

$$|e_i\rangle \otimes |f_j\rangle = |e_i\rangle|f_j\rangle = |e_i, f_j\rangle = |i, j\rangle.$$

Thus,

$$\mathcal{H}_1 \otimes \mathcal{H}_2 = \Big\{ \sum_{i,j} \psi_{i,j} |i, j\rangle \,\Big|\, \psi_{i,j} \in \mathbb{C} \Big\}.$$

We define a scalar product on $\mathcal{H}_1 \otimes \mathcal{H}_2$ by taking these basis elements to be orthonormal:

$$\langle i, j|k, l\rangle = \delta_{i,k}\delta_{j,l}.$$

> The resulting space does not, in fact, depend on the bases $\{e_i\}, \{f_j\}$ used in this construction – but we will not talk about this technical question here.

For two vectors

$$|\alpha\rangle = \sum_i \alpha_i |e_i\rangle \in \mathcal{H}_1, \qquad |\beta\rangle = \sum_j \beta_j |f_j\rangle \in \mathcal{H}_2$$

their tensor product is defined as

$$|\alpha\rangle \otimes |\beta\rangle := \sum_{i,j} \alpha_i \beta_j |i, j\rangle \in \mathcal{H}_1 \otimes \mathcal{H}_2. \tag{1.4}$$

Elements $|\psi\rangle \in \mathcal{H}_1 \otimes \mathcal{H}_2$ whose expansion coefficients *factorize*

$$\psi_{i,j} = \alpha_i \beta_j$$

as in (1.4) are called *product vectors*. All others are called *entangled*. (As you are doubtlessly aware, entanglement is the foundation of many exciting quantum phenomena. We will have more to say about this).

Note that the tensor product space is (by definition) *spanned* by product vectors. Thus, if we want to define an operator on the global space, it suffices to specify how it acts on products. We will use this repeatedly.

> Assume that $\dim \mathcal{H}_i = d_i < \infty$. The a quick parameter counting argument shows that product vectors depend on $d_1 + d_2 - 1$ complex parameters (why the "-1"?), while the tensor product Hilbert space has dimension $d_1 d_2$.
>
> $$\dim \mathcal{H}_1 \otimes \mathcal{H}_2 = d_1 d_2.$$
>
> This suggests (correctly) that "most" elements of $\mathcal{H}_1 \otimes \mathcal{H}_2$ are entangled.

The definition (1.4) implies the "distributive laws"

$$(|\alpha\rangle + |\beta\rangle) \otimes (|\gamma\rangle + |\delta\rangle) = |\alpha\rangle \otimes |\gamma\rangle + |\alpha\rangle \otimes |\delta\rangle + |\beta\rangle \otimes |\gamma\rangle + |\beta\rangle \otimes |\delta\rangle \tag{1.5}$$

and

$$(c|\alpha\rangle) \otimes |\beta\rangle = |\alpha\rangle \otimes (c|\beta\rangle) = c\,(|\alpha\rangle \otimes |\beta\rangle). \tag{1.6}$$

Now let A be an operator on $\mathcal{H}_1$, and B on $\mathcal{H}_2$. Then we define an operator $A \otimes B$ on $\mathcal{H}_1 \otimes \mathcal{H}_2$ via its action on product vectors

$$(A \otimes B)(|\alpha\rangle \otimes |\beta\rangle) = (A|\alpha\rangle) \otimes (B|\beta\rangle).$$

Frequently, we will want to have an operator "act on just one of the factors, leaving the other ones alone". This is done by tensoring with the identity operator $\mathbb{1}$: $A \otimes \mathbb{1}$ or $\mathbb{1} \otimes B$. The $\mathbb{1}$'s are often suppresed, and the factor on which a given operator acts non-trivially is indicated by a sub- or a superscript:

$$A_1 := A^{(1)} := A \otimes \mathbb{1}.$$

We can play this game not just for operators $A : \mathcal{H}_i \to \mathcal{H}_i$, but also for functionals $\mathcal{H}_i \to \mathbb{C}$. For example, if $\langle\gamma|$ is a functional acting on $\mathcal{H}_1$, then

$$\langle\gamma|^{(1)}(|\alpha\rangle \otimes |\beta\rangle) := \langle\gamma|\alpha\rangle\,|\beta\rangle \in \mathcal{H}_2. \tag{1.7}$$

Let's see how these abstract definitions work a bit more concretely. Start with the spin-1/2 Hilbert space $\mathcal{H} \simeq \mathbb{C}^2$ spanned by $|s\rangle$, $s \in \{\pm\frac{1}{2}\}$. The tensor product Hilbert space

$$\mathcal{H}_{1,2} = \mathcal{H}_1 \otimes \mathcal{H}_2 \simeq (\mathbb{C}^2) \otimes (\mathbb{C}^2)$$

of two such spins is indeed spanned by $\{|s_1, s_2\rangle\}$, $s_i \in \{\pm\frac{1}{2}\}$. The observable corresponding to the magnetic quantum number along the z-axis for a single spin is

$$S_z|s\rangle = \hbar s|s\rangle.$$

If we apply that operator to the first spin only, then the rules above give

$$S_z^{(1)}|s_1, s_2\rangle = (S_z \otimes \mathbb{1})|s_1, s_2\rangle = (S_z|s_1\rangle) \otimes (\mathbb{1}|s_2\rangle) = (\hbar s_1|s_1\rangle) \otimes |s_2\rangle = \hbar s_1|s_1, s_2\rangle,$$

i.e. the formal rules of the tensor product reproduce the result we anyway would have guessed. Nice!

The tensor product of $n > 2$ Hilbert spaces $\mathcal{H}_i$ is now defined in the straightforward way:

$$\mathcal{H}_1 \otimes \cdots \otimes \mathcal{H}_n = \bigotimes_{i=1}^{n} \mathcal{H}_i$$

is the space with ONB

$$|e_{i_1}^{(1)}\rangle \otimes \cdots \otimes |e_{i_n}^{(n)}\rangle =: |i_1, \ldots, i_n\rangle, \tag{1.8}$$

where $\{|e_i^{(j)}\rangle\}_i$ is some fixed ONB for the j-th space. While nothing conceptually new happens, it should be remarked that these spaces get *very complicated* very quickly! Consider the simplest case: each $\mathcal{H}_i \simeq \mathbb{C}^2$ describes one spin-1/2. The dimension of the global space is 2^n. For $n \simeq 250$, this exceeds the number of hadrons in the universe. Dealing with this complexity is always non-trivial, and sometimes impossible (this impossibility forming the basis of the power of quantum computers!).

1.1.2 Mixed states

In the introductory QM course, we only considered *pure states*, i.e. preparation procedures of quantum systems that can be described by normalized vectors in the Hilbert space. This notion is not general enough to model all physically relevant situations. As a simple example, consider preparations that are subject to classical uncertainty (c.f. Fig. **??**). Concretely, assume that a pure state $|\psi_i\rangle$ is created with probability q_i. If we measure an observable A, the expected value will be

$$\langle A\rangle = \sum_i q_i \langle\psi_i|A|\psi_i\rangle = \sum_i q_i \operatorname{tr}\big(|\psi_i\rangle\langle\psi_i|A\big) = \operatorname{tr}\Big(\big(\sum_i q_i|\psi_i\rangle\langle\psi_i|\big)A\Big) =: \operatorname{tr}\rho A,$$

where we have defined

$$\rho = \sum_i q_i|\psi_i\rangle\langle\psi_i|. \tag{1.9}$$

Let's collect some properties of ρ. First, $\rho = \rho^\dagger$ because, by by Eq. (A.28), every summand is Hermitian. Next, using the fact that the $|\psi_i\rangle$'s are normalized,

$$\operatorname{tr}\rho = \sum_i q_i \operatorname{tr}|\psi_i\rangle\langle\psi_i| = \sum_i q_i = 1.$$

Thus ρ has unit trace. Finally, for any $|\phi\rangle \in \mathcal{H}$

$$\langle\phi|\rho|\phi\rangle = \sum_i q_i\langle\phi|\psi_i\rangle\langle\psi_i|\phi\rangle = \sum_i q_i|\langle\phi|\psi\rangle|^2 \geq 0.$$

This implies that all eigenvalues of ρ are non-negative. Indeed, if $\{|f_i\rangle\}_i$ are the eigenvectors of ρ, then

$$0 \leq \langle f_j|\rho|f_j\rangle = \langle f_j|\Big(\sum_i \lambda_i|f_i\rangle\langle f_i|\Big)|f_j\rangle = \lambda_j.$$

Hermitian operators with non-negative eigenvalues are called *positive semi-definite* (psd), or sometimes just *positive* for short.

Operators with these three properties have a name: Positive semi-definite trace-one operators are called *density operators*.

We have seen that every "preparation procedure with classical uncertainty" can be modelled by a density operator. What is more, it is an empirical fact that *every* physical preparation procedure of a quantum system can be described by a density operator (ignoring technical difficulties in infinite-dimensional systems). Thus, from now on, by "state", we will mean "density operator".

We collect some definitions and facts (proofs are omitted, but a good exercise!).

A state is called *pure* if it is of the form

$$\rho = |\psi\rangle\langle\psi|$$

for some $|\psi\rangle \in \mathcal{H}$. States that are not pure are called *mixed*. Each of the following conditions is sufficient for a density operator to be pure:

1. $\rho^2 = \rho$,
2. $\operatorname{tr}\rho^2 = 1$,

3. $\operatorname{rank}\rho = 1$.

If each $|\psi_i\rangle = |\psi_i(t)\rangle$ in Eq. (1.9) evolves under the Schrödinger equation, then the density operator ρ satisfies

$$\mathrm{i}\hbar\partial_t\rho(t) = [H, \rho]. \tag{1.10}$$

This is sometimes called the *(quantum) Liouville equation* or the *von Neumann equation*. It is analogous to the equation of motion

$$\partial_t\rho(t) = \{H, \rho\}$$

for a classical probability density ρ on classical phase space, expressed in terms of the Poisson braket. Up to a sign, the Liouville equation is the same as the Heisenberg-picture equation of motion for observables.

We motivated the notion of a mixed state through a *probabilistic* construction – i.e. a process that prepares the state $|\psi_i\rangle\langle\psi_i|$ with probability q_i. As we will see shortly, mixed states also arise in different contexts. This gives rise to intersting quantum phenomena – e.g. *steering* – that are beyond the scope of this course.

For a Hilberst space of dimesnion $d < \infty$, the operator $\frac{1}{d}\mathbb{1}$ can be checked to be a density operator. It is mixed. In fact, it is referred to as the *maximally mixed state* for a number of reasons. The eigenvalues are $\lambda_1 = \cdots = \lambda_d = 1/d$, akin to a *uniform* classical probabilty distribution.

1.1.3 Subsystems and the partial trace

Let

$$\rho = \sum_{i,j;k,l} \rho_{i,j;k,l}|i,j\rangle\langle k,l|$$

be the state of a bi-partite quantum system. Let A be an observable on the first subsystem only. By the discussion above, we know that A acts on the total system as $A \otimes \mathbb{1}$. Thus the expectation value can be written as

$$\langle A\rangle = \operatorname{tr}\Big(\rho\,(A\otimes\mathbb{1})\Big). \tag{1.11}$$

Since we only care about the situation on the fist subsystem, it seems rather wasteful that (1.11) involves the global wave function. It would be nice if there were a density operator

$$\rho^{(1)} = \sum_{i,k} \rho^{(1)}_{i;k}|i\rangle\langle k|$$

on the first system alone such that

$$\langle A\rangle = \operatorname{tr}\Big(\rho\,(A\otimes\mathbb{1})\Big) = \operatorname{tr}\big(\rho^{(1)}A\big). \tag{1.12}$$

To achieve this, define the *partial trace (over the second subsystem)* as

$$\operatorname{tr}_2 : |i,j\rangle\langle k,l| \mapsto |i\rangle\langle k|\,\delta_{j,l}.$$

We claim that

$$\rho^{(1)} = \mathrm{tr}_2\, \rho$$

solves Eq. (1.12). One refers to $\rho^{(1)}$ as the *reduced density operator* or the *marginal state (of the first subsystem)*.

Proof. In terms of the expansion coefficients of ρ, the reduced density matrix reads

$$\begin{aligned}\mathrm{tr}_2\, \rho &= \mathrm{tr}_2 \sum_{i,j,k,l} \rho_{i,j,k,l} |i,j\rangle\langle k,l| \\ &= \sum_{i,k} \sum_{m} \rho_{i,m,k,m} |i\rangle\langle k|\end{aligned}$$

so that

$$\begin{aligned}\mathrm{tr}\left(\rho^{(1)} A\right) &= \sum_{i,k,m} \rho_{i,m,k,m}\, \mathrm{tr}\left(|i\rangle\langle k| A\right) \\ &= \sum_{i,k,m} \rho_{i,m,k,m} \langle k|A|i\rangle \\ &= \sum_{i,k,m} \langle i,m|\rho|k,m\rangle\, \langle k|A|i\rangle \\ &= \sum_{i,m} \langle i,m|\big(\rho(A\otimes \mathbb{1})|i,m\rangle \\ &= \mathrm{tr}\Big(\rho\left(A\otimes\mathbb{1}\right)\Big).\end{aligned}$$

□

As an example, let's look at the *singlet state*

$$|\Psi_-\rangle := \frac{1}{\sqrt{2}}\left(|+,-\rangle - |-,+\rangle\right),$$

known from the theory of coupled spin-1/2's. Expanding $|\Psi_-\rangle\langle\Psi_-|$ and applying the definition of the partial trace, we find

$$\rho^{(1)} = \frac{1}{2}\mathbb{1},$$

where $\mathbb{1}$ is the identity operator on $\mathbb{C}^2$. This is the maximally mixed state from Sec. 1.1.2. Note that the global singlet state is *pure*, and thus the "local" mixedness arises in a way different from the probabilistic construction ("output a pure state according to a classical distribution") encountered before.

1.2 Indistinguishable particles

[This section incorporates material by Johan Aberg.]

It is an empirical fact that the tensor product construction is often not the right description for multi-partite Hilbert spaces. In a way, tensor products are "too big". The physical origin of the problem lies in the fact that two particles of the same type

are *indistinguishable*: E.g., there is no experiment that could tell one electron from another.

This observation is not unique for quantum mechanics. The classical configuration space for, say, two identical particles in one dimension is equally redundant, as the position vectors

$$\begin{pmatrix} q_1 \\ q_2 \end{pmatrix} \qquad \text{and} \qquad \begin{pmatrix} q_2 \\ q_1 \end{pmatrix}$$

describe the same physics. One *could* get rid of this ambiguity, e.g. by specifying only the center of mass $\frac{1}{2}(q_1 + q_2)$ and the *absolute value* of the distance $|q_1 - q_2|$. This would introduce minor technical headaches. (For example, the equations of motion are formulated as differential equations, but the absolute value is not differentiable at $q_1 = q_2$.) One could deal with such problems... but would need to have a good reason for doing so. As no major problems seem to arise from this redundancy, people just never went through the trouble.

> There's *some* indication that things are amiss. The *Gibbs paradox* says that the classical thermodynamical treatment of a gas of identical particles gives the wrong entropy unless indistinguishable configurations are counted only once. However, this doesn't quite falsify the redundant formulation of classical mechanics, as the connection between this microscopic theory and thermodynamics is more tenuous than we would like, and so the problem could lie somewhere else.

In contrast, in quantum mechanics, a failure to treat this redundancy leads to manifestly wrong predictions – e.g. for the theory of atoms with more than one electron (one more reason why we've only treated hydrogen so far).

What is there to do?

In the previous section, we've made a big deal of the fact that we can describe measurments on specific subsystems – for example $X \otimes \mathbb{1}$ vs $\mathbb{1} \otimes X$ for the position of the first and the second particle, respectively. From the discussion above, this is too fine-grained: Any physical measurement procedure that is sensitive to the position of one electron, will happily accept any other electron. Physically well-defined questions inlcude "*Is* there an electron in a given region?" or "*How many* electrons are there in this region?", rather then "*Which* electron is it?". We need to build a theory that allows us to formulate these physical questions only.

There are many different ways of achieving this, and ultimately, it is an empirical question which one is realized in Nature.

The most important approach is to start with a full tensor product Hilbert space (as if the particles were distinguishable), and then to restrict to states that are symmetric under a imagined permutations of the particles. This construction gives rise to *Fermions* and *Bosons* and, as far as we know, accounts for all the elementary particles.

> At this points, many texts offer "proofs" why the construction leading to Fermions and Bosons is the only conceivable way for building a quantum theory of indistinguishable particles. None of these proofs hold up to scrunity. In fact, more general theories *have* been built, e.g. *para-particles* (one simple example will feature in the exercises) and *anyons*. While they don't seem to correspond to any elementary particles, interacting Fermions sometimes allow for an effective description in terms of anyons. Just why people keep perpetuating these arguments is a question I do not know the answer to.

1.2.1 The group of permutations

A permutation π of n letters is a way of re-arranging the symbols $1, 2, \ldots, n$, i.e., π is a bijection of the set $\{1, \ldots, n\}$. There are various ways of denoting permutations. One example is the two-line notation, where the first line contains the numbers $1, \ldots, n$ and the i-th place of the second line is $\pi(i)$

$$\pi = \begin{pmatrix} 1 & 2 & \cdots & n \\ \pi(1) & \pi(2) & \cdots & \pi(n) \end{pmatrix}, \qquad \text{for example} \qquad \begin{pmatrix} 1 & 2 & 3 \\ 2 & 3 & 1 \end{pmatrix}.$$

One can think of this in terms of a graph where arrows point to where each letter is mapped (see Figure 1.1(a)). The set of permutations on n letters forms a group, denoted S_n, and referred to as the *symmetric group*.

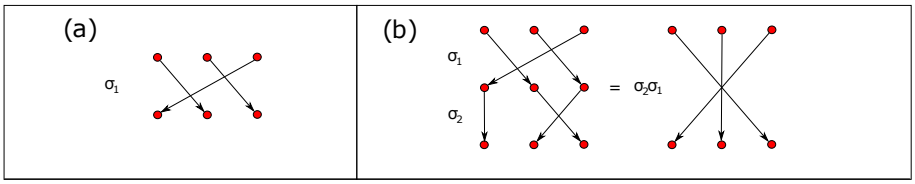

Figure 1.1: (a) A permutation can be regarded as a graph, where each position indicates a letter, and where the arrows points to where each letter is mapped. (b) One can multiply permutations σ_1 and σ_2 by performing one after the other.

How many permutations of n letters are there? Let's count in the two-line notation: There are n ways of chosing the first symobl of the second line, $n-1$ ways of chosing the second symbol (as we can't repeat the first one), etc, for a total of

$$|S_n| = n(n-1)\cdots 2 \cdot 1 = n! \approx e^{n \ln n}.$$

The final estimate is *Stirling's approximation* and shows that there are *many* (super-exponentially many!) permutations.

A *transposition* is a permutation where only two letters are exchanged. Example:

$$\begin{pmatrix} 1 & 2 & 3 & 4 \\ 2 & 1 & 3 & 4 \end{pmatrix}.$$

We will make use of the following facts (that we will not prove):

- Every permutation can be written as a sequence of transpositions.
- For a given permutation, the number of transpositions is either even for all decompositions, or odd for all decompositions.

One may thus define:

$$\mathrm{sgn}(\sigma) = \begin{cases} +1 & \sigma \text{ is product of an even number of transpostions} \\ -1 & \sigma \text{ is product of an odd number of transpositions} \end{cases}$$

You have encountered this definition before, when you learned about the *determinant* of an $(n \times n)$-matrix, which is defined as

$$\det M = \sum_{\pi \in S_n} \mathrm{sgn}(\pi) \prod_{i=1}^{n} M_{i,\pi(i)}. \tag{1.13}$$

Now choose some *single-particle* Hilbert space $\mathcal{H}^{(1)}$ and let

$$\mathcal{H}^{(n)} = \underbrace{\mathcal{H}^{(1)} \otimes \cdots \otimes \mathcal{H}^{(1)}}_{n\times}$$

be the tensor product of n copies of $\mathcal{H}^{(1)}$. We assume some basis $\{|i\rangle\}$ of $\mathcal{H}^{(1)}$ has been fixed, so that the $|i_1, \ldots, i_n\rangle$ form a basis of $\mathcal{H}^{(n)}$ (as in Eq. (1.8)).

If $\pi \in S_n$ is a permutation, it acts on $\mathcal{H}^{(n)}$ by permuting tensor factors

$$\pi : |i_1, \ldots, i_n\rangle \mapsto |\pi(i_1), \ldots, \pi(i_n)\rangle. \tag{1.14}$$

Exercise: Show that (1.14) defines a *unitary* operator.

1.2.2 Bosons

A vector $|\psi\rangle \in \mathcal{H}^{(n)}$ is called *totally symmetric* if

$$\pi|\psi\rangle = |\psi\rangle \qquad \text{for all } \pi \in S_n.$$

Example: For $n = 2$ and single-particle Hilbert space $\mathcal{H}^{(1)}$ spanned by $\{|+\rangle, |-\rangle\}$, each of the *triplet states*

$$|+,+\rangle, \qquad |-,-\rangle, \qquad \frac{1}{\sqrt{2}}(|+,-\rangle + |-,+\rangle), \tag{1.15}$$

is totally symmetric.

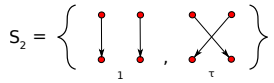

Figure 1.2: S_2 only consists of two elements, the identity 1, and the transposition τ that swaps 1 and 2.

Remember that local observables

$$A^{(i)} = \underbrace{\mathbb{1} \otimes \cdots \otimes \mathbb{1}}_{(i-1)\times} \otimes A \otimes \underbrace{\mathbb{1} \otimes \cdots \otimes \mathbb{1}}_{(n-i)\times} \tag{1.16}$$

– i.e. measurements on one particular particle – were the root of our problems. Our aim now is to find out what happens if one measures one of those on a totally symmetric state vector. To this end, verify that

$$\pi^\dagger A^{(i)} \pi = A^{(\pi^{-1}(i))}.$$

Thus, if $|\psi\rangle$ is totally symmetric, then

$$\begin{aligned} \mathrm{tr}\left(A^{(1)}|\psi\rangle\langle\psi|\right) &= \frac{1}{n!}\sum_{\pi\in S_n} \mathrm{tr}\left(A^{(1)}\pi|\psi\rangle\langle\psi|\pi^\dagger\right) = \frac{1}{n!}\sum_{\pi\in S_n} \mathrm{tr}\left(\pi^\dagger A^{(1)}\pi|\psi\rangle\langle\psi|\right) \\ &= \frac{1}{n}\sum_{i=1}^{n} \mathrm{tr}\left(A^{(i)}|\psi\rangle\langle\psi|\right). \end{aligned} \tag{1.17}$$

Each $A^{(i)}$-measurement just returns the *average of A, taken over all particles*! This *very* promising, as the formalism no longer allows us to pick out the properties of individual particles.

Let

$$\mathrm{Sym}^{(n)}(\mathcal{H}^{(1)}) = \left\{|\psi\rangle \in \mathcal{H}^{(n)} : \pi|\psi\rangle = |\psi\rangle, \quad \forall \pi \in S_n\right\}.$$

be the Hilbert space of all totally symmetric vectors. We define:

- Particles whose n-body Hilbert space is $\mathrm{Sym}^{(n)}(\mathcal{H}^1)$, are called *Bosons*.

At this point of our theory, it is unclear whether Bosons actually exist. But they do. Photons, e.g., are Bosons.

Let's look a bit closer at the Hilbert space of totally symmetric vectors. Define the *symmetrization operator* on $\mathcal{H}^{(n)}$ as

$$P_S : |\psi\rangle \mapsto \frac{1}{n!} \sum_{\pi \in S_n} \pi |\psi\rangle.$$

Exercise: Show that P_S is an orthogonal projection onto $\mathrm{Sym}^{(n)}\left(\mathcal{H}^{(1)}\right)$ and that, hence, the totally symmetric space is spanned by the image $P_S|i_1, \ldots, i_n\rangle$ of a basis under P_S.

Example: Take the basis (1.3) of the tensor product space of two spin-1/2's. The symmetrization operator gives

$$\begin{aligned}
P_S|+,+\rangle &= \frac{1}{2!} \sum_{\pi \in S_2} \pi|+,+\rangle = \frac{1}{2}\big(|+,+\rangle + |+,+\rangle\big) = |+,+\rangle, \\
P_S|+,-\rangle &= \frac{1}{2}(|+,-\rangle + |-,+\rangle), \\
P_S|-,+\rangle &= \frac{1}{2}(|+,-\rangle + |-,+\rangle), \\
P_S|-,-\rangle &= |-,-\rangle.
\end{aligned}$$

We see that the result of the symmetriztion only depends on the number of times each basis vector $|+\rangle, |-\rangle$ appeared in the initial product vector. Also note that the resulting vector is *not* guaranteed to be normalized, even if the initial one was.

In general, the symmetrization

$$P_S|i_1, \ldots, i_n\rangle = \frac{1}{n!} \sum_{\pi \in S_n} |\pi(i_1), \ldots, \pi(i_n)\rangle$$

only depends on the number of times each single-particle basis element appeared in the initial state. This motivates the definition of the *occupation number basis*.

$$\begin{aligned}
|n_1, n_2, \ldots\rangle &:= \sqrt{\frac{n!}{\prod_i n_i!}}\, P_S|\underbrace{1, \ldots, 1}_{n_1 \times}, \underbrace{2, \ldots, 2}_{n_2 \times}, \ldots\rangle, \qquad (1.18) \\
&= \frac{1}{\sqrt{n! \prod_i n_i!}} \sum_{\pi \in S_n} \pi|\underbrace{1, \ldots, 1}_{n_1 \times}, \underbrace{2, \ldots, 2}_{n_2 \times}, \ldots\rangle.
\end{aligned}$$

The funky factorial factor guarantees that the resulting vector is normalized (check it!).

In occupation number notation, the triplet states are

$$\begin{aligned}
|2,0\rangle &= |+,+\rangle, \\
|1,1\rangle &= \frac{1}{\sqrt{2}}\big(|+,-\rangle + |-,\rangle\big), \\
|0,2\rangle &= |-,-\rangle.
\end{aligned}$$

Each element of the occuptation number basis is labeled by a *partition* $n = \sum_{i=1}^{d} n_i$ of n into d non-negative parts. Thus, the dimension of the Bosonic Hilbert space is given by the number of such partitions. There's a cute combinatorial argument for finding it. The answer is

$$\dim \mathrm{Sym}^n\left(\mathbb{C}^d\right) = \binom{n+d-1}{n-1}.$$

If you stare at (1.18), you may be able to find the proof. (Spoiler: Search for "stars and bars").

1.2.3 Fermions

A vector $|\psi\rangle \in \mathcal{H}^{(n)}$ is *totally anti-symmetric* if

$$\pi|\psi\rangle = \mathrm{sgn}(\pi)|\psi\rangle \qquad \forall \pi \in S_n. \tag{1.19}$$

Example: The *singlet*

$$\frac{1}{\sqrt{2}}\big(|+,-\rangle - |-,+\rangle\big)$$

is totally anti-symmetric.

Density matrices that project onto anti-symmetric states are symmetric:

$$\pi^\dagger|\psi\rangle\langle\psi|\pi = \mathrm{sgn}(\pi)^2|\psi\rangle\langle\psi| = |\psi\rangle\langle\psi|.$$

Therefore, the calculation (1.17) holds equally for anti-symmetric $|\psi\rangle$'s! Let

$$\wedge^n(\mathcal{H}^{(1)}) = \left\{|\psi\rangle \in \mathcal{H}^{(n)} : \pi|\psi\rangle = \mathrm{sgn}(\pi)|\psi\rangle\right\}$$

be the Hilbert space of all anti-symmetric vectors (the symbol "$\wedge^n$" is prounounced "*wedge-n*").

- Particles whose n-particle Hilbert space is $\wedge^n(\mathcal{H}^1)$ are called *Fermions*.

Electrons are *Fermions*.

A projection onto the Fermionic n-party space is given by the *anti-symmetrization* operator

$$P_A : |\psi\rangle \mapsto \frac{1}{n!}\sum_{\pi\in S_n} \mathrm{sgn}(\pi)\pi|\psi\rangle.$$

As in the Bosonic case, the Fermionic space is spanned by the image $P_A|i_1,\ldots,i_n\rangle$ of a basis under P_A. Anti-symmetry makes things a bit more exciting, though: If one exchanges two basis vectors (say $i_k \leftrightarrow i_l$) then the anti-symmetrized vector changes sign. This implies that if some basis vector occurs twice ($i_k = i_l$), the anti-symmetrization is equal to 0. Thus the space $\wedge^n\big(\mathcal{H}^{(1)}\big)$ is spanned by

$$\{P_A|i_1,\ldots,i_n\rangle \,|\, i_1 < i_2 < \cdots < i_n\}.$$

and in the Fermionic version

$$|n_1,\ldots,n_d\rangle_{\mathrm{occ}} := \sqrt{n_1!\ldots n_d! n!}\, P_A|\underbrace{1}_{n_1\times},\underbrace{2}_{n_2\times},\ldots,\underbrace{d}_{n_d\times}\rangle,$$

of the occupation number basis (1.18), the occuptation numbers n_i are all either 0 or 1. We have found the *Pauli principle*!

For the anti-symmetrization of a product vector, one also uses the *wedge product notation*

$$P_A\big(|\alpha_1\rangle \otimes |\alpha_2\rangle \otimes \cdots \otimes |\alpha_n\rangle\big) = |\alpha_1\rangle \wedge |\alpha_2\rangle \wedge \cdots \wedge |\alpha_n\rangle,$$

pronounced "*ket alpha one, wedge ket alpha two, wedge...*". For Fermions, the wedge product notation has the advantage over the occupation number notation that one does not have to fix an ordering of the basis vectors to fix the sign. In physics (in particular in quantum chemistry), wedge products are also called *Slater determinants*.

> Indeed, the fact that the *sign* function features both in P_A and in the determinant can be used to establish the following mnemonic for constructing the anti-symmetrization of a product vector $|\alpha_1\rangle \otimes \cdots \otimes |\alpha_n\rangle$ in terms of a formal "*Slater determinant*".
>
> $$P_A\big(|\alpha_1\rangle \otimes \cdots \otimes |\alpha_n\rangle\big) = \frac{1}{n!} \det \begin{pmatrix} \alpha_1^{(1)} & \alpha_2^{(1)} & \dots & \alpha_n^{(1)} \\ \alpha_1^{(2)} & \alpha_2^{(2)} & \dots & \alpha_n^{(2)} \\ \vdots & \vdots & & \vdots \\ \alpha_1^{(n)} & \alpha_2^{(n)} & \dots & \alpha_n^{(n)} \end{pmatrix}.$$
>
> Here, the super-scripts indicate which tensor factor the vector belongs to. In reference to this construction, anti-symmetrized products are often called *Slater determiants*.

1.2.4 Non-Interacting Particles

A significant part of physics consists of mapping a given many-body Hamiltonian to one of the form "non-interacting particles + small perturbation term".

An n-particle system is *non-interacting* if the Hamiltonian is of the form

$$H = \sum_{j=1}^{n} H_0^{(j)},$$

where $H_0^{(i)}$ is some fixed single-body Hamiltonian H_0 acting on the i-th particle as in Eq. (1.16). To solve the stationary Schrödinger equation of non-interacting systems, it suffices if one can solve the single-particle Hamiltonian H_0. Indeed, assume that $H_0|E_i\rangle = E_i|E_i\rangle$ with the eigenvalues $E_0, E_1, \dots$ ordered non-decreasingly.

Fermions: For $i_1 < i_2 < \cdots < i_n$, one can easily check

$$\begin{aligned} H\left(|E_{i_1}\rangle \wedge |E_{i_2}\rangle \wedge \cdots \wedge |E_{i_n}\rangle\right) &= \sum_j H_0^{(j)}\big(|E_{i_1}\rangle \wedge |E_{i_2}\rangle \wedge \cdots \wedge |E_{i_n}\rangle\big) \\ &= \big(E_{i_1} + \cdots + E_{i_n}\big)\left(|E_{i_1}\rangle \wedge |E_{i_2}\rangle \wedge \cdots \wedge |E_{i_n}\rangle\right). \end{aligned}$$

Thus, Slater determinants formed from single-body eigenstates are eigenvectors of the n-Fermion Hamiltonian. Because they form a basis of $\wedge^n\big(\mathcal{H}^{(1)}\big)$, we obtain all eigenvalues and eigenfunctions this way. The eigenvalues are exactly the sums over subsets

of n eigenvalues of the single-particle Hamiltonian. In particular, the groundstate and ground state energy are

$$|E_0\rangle \wedge |E_{i_2}\rangle \wedge \cdots \wedge |E_{i_{n-1}}\rangle, \qquad E_0 + E_1 + \cdots + E_{n-1}.$$

The highest energy E_{n-1} that is still occupied in such a Slater determinant is called the *Fermi energy*.

Bosons: Arguing as above, the occupation number states, formed by symmetrizing single-body eigenvectors, form a complete eigenbasis:

$$H|n_1, \ldots, n_d\rangle = \big(\sum_i E_i n_i\big)|n_1, \ldots, n_d\rangle.$$

In particular, the ground state of n Bosons is nE_0.

1.2.5 Two electron systems and the exchange interaction

[Following Ballentine. See Mattis, *The Theory of Magnetism I* for more thorough treatment.]

We consider the effect of the anti-symmetrization postulate on two electrons.

The Hilbert space of each electron is

$$\mathcal{H}^{(1)} = L^2(\mathbb{R}^3) \otimes \mathbb{C}^2,$$

where the first tensor factor encodes the three motional degrees of freedom, and the second factor, with basis $\{|+\rangle, |-\rangle\}$, represents the spin-$1/2$ degree of freedom. In other words, $\mathcal{H}^{(1)}$ has a basis

$$|\vec{x}, s\rangle, \qquad \vec{x} \in \mathbb{R}^3, \quad s \in \{\pm 1/2\}$$

labeled by position and spin eigenvectors, and a general state vector $|\psi\rangle \in \mathcal{H}^{(1)}$ of an electron can be described by a "wave function"

$$\psi(\vec{x}, s) = \langle \vec{x}, s|\psi\rangle, \qquad \vec{x} \in \mathbb{R}^3, \quad s \in \{\pm 1/2\}$$

that depends both on the position and on the spin variables.

Now consider the tensor product $\mathcal{H}^{(2)}$ of two electron Hilbert spaces. The permutation operator τ interchanges both the spatial and the spin degrees of freedom:

$$\tau\,|\vec{x}_1, s_1, \vec{x}_2, s_2\rangle = |x_2, s_2, x_1, s_1\rangle, \quad \text{or} \quad (\tau\psi)(\vec{x}_1, s_1, \vec{x}_2, s_2) = \psi(\vec{x}_2, s_2, \vec{x}_1, s_1).$$

It turns out to be a good idea to look for anti-symmetric vectors $|\psi\rangle$ of the form

$$\psi(\vec{x}_1, s_1, \vec{x}_2, s_s) = \phi(\vec{x}_1, \vec{x}_2)\chi(s_1, s_2), \tag{1.20}$$

where either ϕ is symmetric and χ anti-symmetric, or vice versa.

> In fact, this is no loss of generality, as vectors of the form (1.20) span the Fermionic Hilbert space. This is not difficult to prove – try it!

Consider two protons at fixed positons $\vec{r}_A, \vec{r}_B$. We aim to analyze the Hamiltonian

$$\begin{aligned} H &= H_0 + V, \\ H_0 &= \sum_{i=1}^{2} \left(-\frac{\hbar^2}{2m}\Delta_1 - \frac{e^2}{4\pi\epsilon_0 \|\vec{x}_i - \vec{r}_A\|} - \frac{e^2}{4\pi\epsilon_0 \|\vec{x}_i - \vec{r}_B\|} \right), \\ V &= \frac{e^2}{4\pi\epsilon_0 \|\vec{x}_1 - \vec{x}_2\|} \end{aligned}$$

of two electrons, interacting with the protons and themselves via the Coulomb potential. Here,

$$\Delta_i = \partial_{x_i}^2 + \partial_{y_i}^2 + \partial_{z_i}^2$$

is the Laplace operator acting on the position of the i-th particle. Note that the spin does *not* enter this Hamiltonian directly.

Recall that the eigenfunctions ϕ_{nlm} of a hydrogen atom centered at the origin are labeled by quantum numbers

$$n \in \mathbb{N}, \quad 0 \leq l \leq n-1, \quad -l \leq m \leq l.$$

To describe the spatial part of the electron wave functions, we will work with the "doubled" set

$$\phi_{nlm}^{(A)}(\vec{x}) := \phi_{nlm}(\vec{x} - \vec{r}_A), \qquad \phi_{nlm}^{(B)}(\vec{x}) := \phi_{nlm}(\vec{x} - \vec{r}_B)$$

of hydrogen solutions, centered at $\vec{r}_A$ and $\vec{r}_B$ respectively. These wave functions are *not* orthogonal – but, as the radial part of the ϕ_{nlm} decreases exponentially with r, they are "almost orthogonal" if $\|\vec{r}_A - \vec{r}_B\|$ is big enough (Fig. **??**).

Assume first that the atoms are so far apart that the interaction term V can be neglected (why is this possible?). Then (up to exponentially small corrections, see above), the ground state space is spanned by the four Slater determinants

$$|\phi_{100}^{(A)}, s_A\rangle \wedge |\phi_{100}^{(B)}, s_B\rangle \qquad s_A, s_B \in \{\pm 12\} \tag{1.21}$$

with energy $-2E_I$, twice the ionization energy of hydrogen.

Now decrease the distance such that $|\langle \phi_{100}^{(A)} | \phi_{100}^{(B)} \rangle|$ becomes appreciable, but $|\langle \phi_{100}^{(A)} | \phi_{100}^{(B)} \rangle|^2$ can still be neglected. The repulsive interaction term V becomes relevant. Physically, we may expect this to happen: It should be energetically favorable if the spin component $\chi(s_A, s_B)$ of the wave function is symmetric, as this forces the spatial component to be anti-symmetric, which in turn "decreases the probability of the two electrons being close to each other".

To get a quantitative prediction, we compute the eigenvalues of the full Hamiltonian restricted to the space (1.21). (This is an approximation: The real ground state vector will contain contributions from spatial wave functions ϕ_{nlm} with higher energies.) Since the Hamiltonian does not directly depend on the spin degrees of freedom, the energy on the space (1.21) is a function only of the symmetry class. We thus set

$$\phi_{\pm}(\vec{x}_1, \vec{x}_2) = \frac{1}{\sqrt{2}} \big(\phi_{100}^{(A)}(\vec{x}_1) \phi_{100}^{(B)}(\vec{x}_2) \pm \phi_{100}^{(A)}(\vec{x}_2) \phi_{100}^{(B)}(\vec{x}_1) \big)$$

and determine

$$E_\pm = \frac{\langle\phi_\pm|H|\phi_\pm\rangle}{\langle\phi_\pm|\phi_\pm\rangle} = \frac{\langle\phi_\pm|H|\phi_\pm\rangle}{1 \pm |\langle\phi_{100}^{(A)}|\phi_{100}^{(B)}\rangle|^2} \approx \langle\phi_\pm|H|\phi_\pm\rangle.$$

Compute:

$$\begin{aligned}
&E_+ + E_- \\
=&\langle\phi_+|H|\phi_+\rangle + \langle\phi_-|H|\phi_-\rangle = \langle\phi_+|V|\phi_+\rangle + \langle\phi_-|V|\phi_-\rangle \\
=&2\frac{e^2}{4\pi\epsilon_0}\int \mathrm{d}^3\vec{x}_1 \int \mathrm{d}^3\vec{x}_2\, \bar{\phi}_{100}^{(A)}(\vec{x}_1)\bar{\phi}_{100}^{(B)}(\vec{x}_2)\frac{1}{\|\vec{x}_1 - \vec{x}_2\|}\phi_{100}^{(A)}(\vec{x}_1)\phi_{100}^{(B)}(\vec{x}_2), \\
=&2\frac{e^2}{4\pi\epsilon_0}\int \mathrm{d}^3\vec{x}_1 \int \mathrm{d}^3\vec{x}_2\, |\phi_{100}^{(A)}(\vec{x}_1)|^2|\phi_{100}^{(B)}(\vec{x}_2)|^2\,\frac{1}{\|\vec{x}_1 - \vec{x}_2\|} =: 2I,
\end{aligned}$$

$$\begin{aligned}
&E_+ - E_- \\
=&2\frac{e^2}{4\pi\epsilon_0}\int \mathrm{d}^3\vec{x}_1 \int \mathrm{d}^3\vec{x}_2 \bar{\phi}_{100}^{(A)}(\vec{x}_1)\bar{\phi}_{100}^{(B)}(\vec{x}_2)\frac{1}{\|\vec{x}_1 - \vec{x}_2\|}\phi_{100}^{(A)}(\vec{x}_2)\phi_{100}^{(B)}(\vec{x}_1) =: 2J.
\end{aligned}$$

These integrals, which we will not evaluate explicitly, are called the *direct integral* I and the *exchange integral* J, respectively. Because ϕ_{100} can be represented as a positive function, both I and J are positive. The result of the interaction is therefore to increase the mean energy by I and also to introduce an energy splitting of magnitude $2J$ between the symmetric and the anti-symmetric solutions (Fig. **??**).

The Heisenberg model: The formally degenerate ground state space depends only on the spin configuration. Let's map it to an effective 2-spin model by setting:

$$|s_1, s_2\rangle := |\phi_{100}^{(A)}, s_1\rangle \wedge |\phi_{100}^{(B)}, s_2\rangle$$

(that's how one recovers effectively distinguishable particles from Fermions...). In this two-spin Hilbert space, the effective Hamiltonian is

$$H_{\text{eff}} = -J\tau.$$

We can write the transposition τ as (excercise!)

$$\tau = \sum_{j\in 0,x,y,z} \sigma_j^{(1)}\sigma_j^{(2)} = \mathbb{1} + \vec{\sigma}^{(1)} \cdot \vec{\sigma}^{(2)}$$

and thus, up to an global shift of the energies,

$$H_{\text{eff}} = -J\,\vec{\sigma}^{(1)} \cdot \vec{\sigma}^{(2)}. \tag{1.22}$$

The exchange principle can thus be described as an effective interaction between the two spins. Equation (1.22) is an embryonic version of the *Heisenberg model* of magnetism.

Similar techniques can be used for estimating the energies of the Helium atom [C.f. Ballentine, Rae, and in particular, Cohen-Tannoudji].

1.2.6 Boson Sampling

TBD.

1.3 Fock space and "second quantization"

So far, we have considered systems with a fixed number n of particles. We will now treat the particle number as another variable. Mathematically, this actually simplifies some calculations. Physically, this step is necessary e.g. for relativistic quantum field theories, where different species of particles can be converted into each other.

1.3.1 Bosons

Fix some single-body Hilbert space $\mathcal{H}^{(1)}$ with basis $\{|i\rangle\}_i$. We need to include the possibility $n = 0$ of "no particles" in our description. To this end, define

$$\mathrm{Sym}^{(0)}(\mathcal{H}^{(1)}) = \mathbb{C}$$

and denote the basis "vector" $1 \in \mathbb{C}$ as $|\,\mathrm{vac}\rangle$. The *(symmetric) Fock space* over $\mathcal{H}^{(1)}$

$$\mathcal{F}_S\big(\mathcal{H}^{(1)}\big) = \bigoplus_{n=0}^{\infty} \mathrm{Sym}^n(\mathcal{H}^{(1)})$$

is the Hilbert space of vectors of the form

$$\begin{aligned}|\psi\rangle &= |\,\mathrm{vac}\rangle + \sum_{i_1} c_{i_1}|i_1\rangle + \sum_{i_1,i_2} c_{i_1 i_2} P_S|i_1,i_2\rangle + \dots \\ &= \sum_{n=0}^{\infty} \sum_{i_1,\dots,i_n} c_{i_1,\dots,i_n} P_S|i_1,\dots,i_n\rangle.\end{aligned}$$

Things are simpler in the occupation number basis, where a general element of the Fock space takes the form

$$|\psi\rangle = \sum_{n_1,n_2,\dots=0}^{\infty} c'_{n_1,n_2\dots}|n_1,n_2,\dots\rangle_{\mathrm{occ}}.$$

Creation and annihilation operators: We usually avoid writing out a Fock space vector directly, but instead describe them using the hugely important formalism of creation and annihilation operators. With any element $|\alpha\rangle \in \mathcal{H}^{(1)}$ of the single-body Hilbert space, we associate a *creation operator* which maps $\mathrm{Sym}^n(\mathcal{H}^{(1)}) \to \mathrm{Sym}^{n+1}(\mathcal{H}^{(1)})$ by

$$a^\dagger_{|\alpha\rangle}|\psi\rangle = \sqrt{n+1}\, P_S\big(|\alpha\rangle \otimes |\psi\rangle\big). \tag{1.23}$$

If basis is fixed, we set $a_i^\dagger := a^\dagger_{|i\rangle}$. In occupation number picture:

$$a_i^\dagger|n_1,n_2,\dots,\rangle_{\mathrm{occ}} = \sqrt{n_i+1}|n_1,n_2,\dots,n_{i-1},n_i+1,n_{i+1},\dots\rangle_{\mathrm{occ}} \tag{1.24}$$

(the normalization constant follows from (1.18)). The adjoint $a_{|\alpha\rangle} = \big(a^\dagger_{|\alpha\rangle}\big)^\dagger$ is called the *annihilation operator*[1]. From (1.24),

$$\begin{aligned}\sqrt{n_i+1}\delta_{n_i',n_i+1}\prod_{j\neq i}\delta_{n_j,n_j'} &= \langle n_1',\dots|a_i^\dagger|n_1,\dots\rangle \\ &= \langle n_1,\dots|a_i|n_1',\dots\rangle^* = \sqrt{n_i'}\delta_{n_i'-1,n_i}\prod_{j\neq i}\delta_{n_j',n_j},\end{aligned}$$

hence

$$a_i|n_1,n_2,\dots\rangle_{\rm occ} = \sqrt{n_i}|n_1,n_2,\dots,n_{i-1},n_i-1,n_{i+1},\dots\rangle_{\rm occ}.$$

(Remember: "square root of larger number"). Because

$$a_i^\dagger a_i|n_1,\dots,\rangle = n_i|n_1,\dots,\rangle,$$

the operator $N_i = a_i^\dagger a_i$ is called the *number operator*.

Basis change: Let

$$|\alpha\rangle = \sum_i c_i|i\rangle \in \mathcal{H}^{(1)}.$$

Using (1.23),

$$a^\dagger_{|\alpha\rangle}|\psi\rangle = \sqrt{n+1}P_S\big(|\alpha\rangle\otimes|\psi\rangle\big) = \sqrt{n+1}\sum_i P_S\big(c_i|i\rangle\otimes|\psi\rangle\big) = \sum_i c_i\, a_i^\dagger|\psi\rangle,$$

so that

$$a^\dagger_{|\alpha\rangle} = \sum_i c_i\, a_i^\dagger = \sum_i \langle i|\alpha\rangle\, a_i^\dagger, \qquad a_{|\alpha\rangle} = \sum_i \overline{c_i}\, a_i = \sum_i \langle\alpha|i\rangle\, a_i. \tag{1.25}$$

Commutation relations: The Bosonic creation and annihilation operators fulfill these basic communtation relations:

$$[a_i, a_j^\dagger] = \delta_{ij}\mathbb{1}, \qquad [a_i,a_j] = [a_i^\dagger,a_j^\dagger] = 0. \tag{1.26}$$

More generally, plugging (1.25) into (1.26) gives

$$[a_{|\alpha\rangle}, a^\dagger_{|\beta\rangle}] = \langle\alpha|\beta\rangle\ \mathbb{1}. \tag{1.27}$$

Field operators: It is beneficial to apply the above formalism also to generalized bases labeled by continuous parameters. The most imporantly examples are, of course, the Dirac delta functions $|\vec{x}\rangle$ and the momentum eigenstates $|\vec{k}\rangle$ with

$$\phi_{\vec{k}}(\vec{x}) = (2\pi)^{-3/2}e^{\mathrm{i}\vec{k}\vec{x}}.$$

[1] It is somewhat unfortunate that $a^\dagger$ is a more natural starting point than a, and that $a_{|\alpha\rangle}$ depends *anti*-linearly on $|\alpha\rangle$, and $a^\dagger_{|\alpha\rangle}$ linearly. Well, at least it means that one can easily remember the action of the operators, as physicists use the "dagger" symbol † to denote the adjoint, and † looks a bit like a +-sign, which conveniently goes with the operator that adds a particle.

For example, if $\{|\phi_i\rangle\}_i$ labels a countable basis of smooth functions $\phi_i \in L^2(\mathbb{R}^3)$, Eq. (1.25) gives

$$a^\dagger_{\vec{x}} = \sum_i \bar{\phi}_i(\vec{x}) a^\dagger_i, \qquad a^\dagger_{|\phi_i\rangle} = \int \mathrm{d}^3\vec{x}\, \phi_i(\vec{x}) a^\dagger_{\vec{x}}, \tag{1.28}$$

the relation between position basis and momentum basis is

$$a^\dagger_{\vec{k}} = (2\pi)^{-3/2} \int e^{\mathrm{i}\vec{k}\vec{x}} a^\dagger_{\vec{x}}\, \mathrm{d}^3\vec{x}, \qquad a^\dagger_{\vec{x}} = (2\pi)^{-3/2} \int e^{-\mathrm{i}\vec{k}\vec{x}} a^\dagger_{\vec{x}}\, \mathrm{d}^3\vec{k}, \tag{1.29}$$

and (1.27) becomes

$$[a_{\vec{x}}, a^\dagger_{\vec{y}}] = \delta(x-y)\, \mathbb{1}. \tag{1.30}$$

As discussed in more detail in Sec. A.1.4, there are various ways of making sense of these expressions. The cleanest approach is

- *Integrate against smooth functions*: Eq. (1.30) can be read as a short-hand way of saying that for smooth functions α, β, it holds that

$$\begin{aligned}
[a_{|\alpha\rangle}, a^\dagger_{|\beta\rangle}] &= \int\int \bar{\alpha}(\vec{x})\beta(\vec{y})[a_{\vec{x}}, a^\dagger_{\vec{y}}]\, \mathrm{d}^3\vec{x}\, \mathrm{d}^3\vec{y} \\
&= \int\int \bar{\alpha}(\vec{x})\beta(\vec{y})\delta(\vec{x}-\vec{y})\, \mathbb{1}\, \mathrm{d}^3\vec{x}\, \mathrm{d}^3\vec{y} \\
&= \int \bar{\alpha}(\vec{x})\beta(\vec{y})\mathbb{1}\, \mathrm{d}^3\vec{y} \\
&= \langle\alpha|\beta\rangle\, \mathbb{1},
\end{aligned} \tag{1.31}$$

  which is just the unproblematic version (1.27) for proper functions.

Creation and annihilation operators for Dirac delta functions are called *field operators* and written as

$$\Psi(\vec{x}) := a_{|\vec{x}\rangle}, \qquad \Psi^\dagger(\vec{x}) := a^\dagger_{|\vec{x}\rangle}.$$

We can now explain the name *second quantization* for the process of passing from a single-party Hilbert space to Fock space. As we will see momentarily, if one writes out symmetrized single-body observables in terms of field operators, one gets expressions that formally looks like a a single-body expectation value, but where the wave function has been replaced by a field operator. For example, let Q_R be the projection operator onto wave functions supported on some region $R \subset \mathbb{R}^3$, i.e.

$$(Q_R\psi)(\vec{x}) = \begin{cases} \psi(x) & \vec{x} \in R \\ 0 & \text{else} \end{cases}.$$

In single-particle QM, the probability of finding the particle in R is $\langle\psi|Q_R|\psi\rangle$, or

$$\int_R \mathrm{d}^3\vec{x}\, \overline{\psi}(x)\psi(x). \qquad \text{(an expectation value)}$$

On the other hand, the symmetrized observable $P_S Q_R P_S$ can be written as

$$\int_R \mathrm{d}^3\vec{x}\, \Psi^\dagger(\vec{x})\Psi(\vec{x}). \qquad \text{(an observable)}$$

It looks like "the wave function has been replaced by operators that fulfill the canonical communtation relations (1.30)". Because, as we will see, a similar substitution occurs when passing from classical to quantum fields, one may think that by working on Fock space, single-particle QM has been "quantized again". However, the analogy to field quantization is imperfect, so one should not take the term too seriously.

Connection with harmonic oscilllator: Recall that creation and annihilation operators first occured in the analysis of the quatnum harmonic oscillator, where they were defined in terms of the position and momentum operators as

$$a = \frac{1}{\sqrt{2}}(X + iP), \qquad a^\dagger = \frac{1}{\sqrt{2}}(X - iP).$$

They act as ladder operators on the eigenbasis $\{|n\rangle\}_{n=0}^\infty$ of

$$H_{\text{ho}} = \frac{1}{2}\hbar\omega(P^2 + X^2) = \hbar\omega(a^\dagger a + 1/2).$$

The similarity in notation between the "harmonic oscillator ladder operators and energy eigenstates" and their many-body versions is no coincidence. If we identify the single-party Hilbert space $L^2(\mathbb{R})$ of the harmonic oscillator with the Fock space over $\mathcal{H}^{(1)} = \mathbb{C}$ via

$$L^2(\mathbb{R}) \to \mathcal{F}_S(\mathbb{C}), \qquad |n\rangle_{\text{ho}} \mapsto |n\rangle_{\text{occ}}$$

then, under the same identification, $a^\dagger_{\text{ho}} \mapsto a^\dagger_{\text{Fock}}$. Up to the constant term $\hbar\omega/2$, the harmonic oscillator Hamiltonian H_{ho} maps to the non-interacting Boson model with single-body Hamiltonian $H_0 = \hbar\omega$ (a "one-by-one matrix").

So we can think about the Harmonic oscillator either as single-body infinite-dimensional system, or as an infinite-particle Bosonic Fock space over a one-dimensional Hilbert space.

1.3.2 Fermions

The Fermionic version proceeds analogously:

$$\mathcal{F}_A\big(\mathcal{H}^{(1)}\big) = \bigoplus_{n=0}^\infty \wedge^n(\mathcal{H}^{(1)})$$

is the Hilbert space of vectors of the form

$$\begin{aligned}|\psi\rangle &= |\,\text{vac}\rangle + \sum_{i_1} c_{i_1}|i_1\rangle + \sum_{i_1<i_2} c_{i_1 i_2} P_A|i_1, i_2\rangle + \dots \\ &= \sum_{n=0}^\infty \sum_{i_1<\dots<i_n} c_{i_1,\dots,i_n} P_A|i_1, \dots, i_n\rangle.\end{aligned}$$

If the single-party Hiblert space is d-dimensional, then the direct sum of Fock space terminates after d summands. The creation and annihilation operators on $\wedge^n\big(\mathcal{H}^{(1)}\big)$ are defined via

$$a^\dagger_{|\alpha\rangle}|\psi\rangle = \sqrt{n+1}P_A\big(|\alpha\rangle \otimes |\psi\rangle\big). \tag{1.32}$$

and fulfill

$$a_i^\dagger |n_1, \dots, n_i, \dots\rangle = (-1)^{\sum_{j<i} n_j} |n_1, \dots, n_i + 1, \dots\rangle,$$

and

$$\{a_i, a_j^\dagger\} = \delta_{ij}\mathbb{1}, \qquad \{a_i, a_j\} = \{a_i^\dagger, a_j^\dagger\} = 0, \tag{1.33}$$

where the braces denote the *anti-commutator* $\{A, B\} = AB + BA$.

Parity superselection rule: The fact that ladder operatators corresponding to orthogonal single-particle states *anti*-commute is a potential source of trouble! Indeed, consider a many-Fermion system. Choose two widely separated regions $A, B \subset \mathbb{R}^3$ and vectors $|\alpha\rangle, |\beta\rangle \in L^2(\mathbb{R}^3)$ that are supported in A, B respectively (Fig. **??**). Assume the system is in the state

$$|\psi\rangle = \frac{1}{\sqrt{2}}\big(|\text{vac}\rangle + |\beta\rangle\big) \in \mathcal{F}_A\big(L^2(\mathbb{R})\big),$$

a super-position of the vaccum and a particle located in region B. The operators

$$O_A := a_{|\alpha\rangle} + a_{|\alpha\rangle}^\dagger, \qquad O_B := a_{|\beta\rangle} + a_{|\beta\rangle}^\dagger$$

are both unitary and Hermitian (why?). By the commutation relations (1.33),

$$\begin{aligned} O_A^\dagger O_B O_A &= (a_\alpha + a_\alpha^\dagger)(a_\beta + a_\beta^\dagger)(a_\alpha + a_\alpha^\dagger) = -(a_\beta + a_\beta^\dagger)(a_\alpha + a_\alpha^\dagger)(a_\alpha + a_\alpha^\dagger) \\ &= -O_B O_A^\dagger O_A = -O_B. \end{aligned}$$

Assume that Alice has access to region A and can decide to apply the unitary O_A to the quantum system (what does that *mean*?). Assume that Bob has access to region B and measures the observable O_B. If Alice does not apply her unitary, the expectation value of Bob's measurement in a state $|\psi\rangle$ is

$$\langle\psi|O_B|\psi\rangle = \frac{1}{2}.$$

But if she *does* apply O_A, the expectation value changes to

$$\langle\psi|O_A^\dagger O_B A_B|\psi\rangle = -\langle\psi|O_B|\psi\rangle = -\frac{1}{2}.$$

Thus the decision of Alice can have immediate detectable consequences for Bob – even though they are, by assumption, widely separated. This is incompatible with the *microcausality principle*, which posits that local actions should not have immediate consequences over arbitrarily large distances. Thus, our current theory of Fermions is "too large": It allows us to formalize unphysical scenarios. We thus have to restrict the set of operators or states that we consider physical. Such restrictions are called *super-selection rules*. For Fermions, it turns out that the *parity super-selection rule* gets rid of the violations of micro-causality, while still allows us to describe all known phenomena. There are many equivalent ways of stating it. One is to demand that physical operators can always be written as the sum over products of ladder operators involving an *even number of factors*. In this way, factors of -1 always occur and even number of times and hence cancel.

1.3.3 Symmetrized operators

Let

$$A = \sum_{ij} A_{ij} |i\rangle\langle j| = \sum_{ij} \big(\langle i|A|j\rangle\big)\, |i\rangle\langle j|$$

be a single-particle operator. To work with n indistinguishable particles, we need to map A to the symmetrized version $A^{(1)} + \cdots + A^{(n)}$, and, on Fock space,

$$A \mapsto \bigoplus_{n=1}^{\infty} \sum_{k=1}^{n} A^{(k)}. \tag{1.34}$$

We claim that for both Bosons and Fermions, the following convenient formula holds

$$\bigoplus_{n=1}^{\infty} \sum_{k=1}^{n} A^{(k)} = \sum_{ij} A_{ij}\, a_i^\dagger a_j.$$

In other words: We can formally move from single-body operators to many-body operators replacing "ket's by creation operators and bra's by annihilation operators".

Proof. Assume that $A = A^\dagger$ is Hermitian with eigendecomposition

$$A = \sum_i \lambda_i |\phi_i\rangle\langle\phi_i|.$$

If we form the occupation number basis in terms of the eigenbasis $\{|\phi_i\rangle\}_i$ and set $b_i := a_{|\phi_i\rangle}$, then the calculation done in Section 1.2.4) showes that

$$\big(\sum_{k=1}^{n} A^{(k)}\big)|n_1, \ldots\rangle_{\text{occ}} = \sum_i \lambda_i n_i |n_1, \ldots\rangle_{\text{occ}} = \sum_i \lambda_i b_i^\dagger b_i |n_1, \ldots\rangle_{\text{occ}}$$

which implies equality of the operators. Using the transformation laws of ladder operators,

$$\sum_i \lambda_i b_i^\dagger b_i = \sum_{ikl} \lambda_i \langle k|\phi_i\rangle\langle\phi_i|l\rangle a_k^\dagger a_l. \tag{1.35}$$

At the same time,

$$A = \sum_i \lambda_i |\phi_i\rangle\langle\phi_i| = \sum_{ikl} \lambda_i \langle k|\phi_i\rangle\langle\phi_i|l\rangle\, |k\rangle\langle l|. \tag{1.36}$$

Comparing (1.35) with (1.36) gives the result for Hermitian operators. But then it holds generally, as any operator can be writte as a linear combination

$$A = \frac{1}{2}(A + A^\dagger) + \frac{1}{2}(A - A^\dagger) = \frac{1}{2}(A + A^\dagger) - i\frac{i}{2}(A - A^\dagger)$$

(possibly with complex coefficients) of Hermitian ones. □

Likewise, if A is a two-body operator on $\mathcal{H}^{(1)} \otimes \mathcal{H}^{(2)}$, then the symmetrized n-body version is

$$\frac{1}{2} \sum_{i=1}^{n} \sum_{i \neq j=1}^{n} A^{(i,j)},$$

where the super-script denotes the two particles on which the operator acts non-trivially. The factor $1/2$ is there to avoid double-counting of (i, j) and (j, i). As above, one can show that

$$\frac{1}{2} \bigoplus_{n=1}^{\infty} \sum_{i=1}^{n} \sum_{i \neq j=1}^{n} A^{(i,j)} = \frac{1}{2} \sum_{ijkl} V_{ijkl}\, a_i^\dagger a_j^\dagger a_l a_k, \qquad V_{ijkl} = \langle ij|V|kl\rangle.$$

Note that the indices l, k of the annihilation operators are *reversed* as compared to the indices in the matrix element! We omit the proof.

Common single-body terms: Some formulas are taken from Sec. A.1.4.

- The potential operator

  $$V = \int v(\vec{x}) |\vec{x}\rangle\langle\vec{x}| \, \mathrm{d}^3\vec{x}$$

  maps to

  $$\int v(\vec{x}) a_{\vec{x}}^\dagger a_{\vec{x}} \mathrm{d}^3\vec{x} = \int v(\vec{x}) \Psi^\dagger(\vec{x}) \Psi(\vec{x}) \, \mathrm{d}^3\vec{x}.$$

- The momentum operator

  $$P = -i \int \hbar\vec{k} \, |\vec{k}\rangle\langle\vec{k}| \, \mathrm{d}^3\vec{k}$$

  becomes

  $$-i \int \hbar\vec{k} \, a_{\vec{k}}^\dagger a_{\vec{k}} \, \mathrm{d}^3\vec{k}.$$

  In the sense of Sec. A.1.4, one can also write the momentum operator in position basis as

  $$P = -i\hbar \int \Psi^\dagger(\vec{x}) \, \vec{\nabla} \, \Psi(\vec{x}) \, \mathrm{d}^3\vec{x}. \tag{1.37}$$

  As always (Sec. A.1.4), Eq. (1.37) is justified as it gives the right expression when expressed in a smooth basis. Let's check this in the momentum basis, where (1.29) gives

  $$\begin{aligned}
  &- i\hbar \int \Psi^\dagger(\vec{x}) \vec{\nabla} \Psi(\vec{x}) \, \mathrm{d}^3\vec{x} \\
  &= - i\hbar (2\pi)^{-3} \int e^{-i\vec{k}\vec{x}} a_{\vec{k}}^\dagger \vec{\nabla} e^{i\vec{k}'\vec{x}} a_{\vec{k}'} \, \mathrm{d}^3\vec{k} \mathrm{d}^3\vec{k}' \mathrm{d}^3\vec{x} \\
  &= - i\hbar \int (i\vec{k}') a_{\vec{k}}^\dagger a_{\vec{k}'} (2\pi)^{-3} \int e^{i(\vec{k}'-\vec{k})\vec{x}} \, \mathrm{d}^3\vec{k} \mathrm{d}^3\vec{k}' \mathrm{d}^3\vec{x} \\
  &= \int \hbar\vec{k} \, a_{\vec{k}}^\dagger a_{\vec{k}} \, \mathrm{d}^3\vec{k},
  \end{aligned}$$

  as it should.

- The kinetic energy term reads

$$(2\pi)^{-3}\int \frac{\hbar^2\|\vec{k}\|^2}{2m}a^\dagger_{\vec{k}}a_{\vec{k}}\,\mathrm{d}^3\vec{k}.$$

Interaction potential: Let

$$V|\vec{x}_1,\vec{x}_2\rangle = v(\vec{x}_2-\vec{x}_1)|\vec{x}_1,\vec{x}_2\rangle$$

be an interaction term that only depends on the relative position of two particles. The most prominent example is, of course, the Coulomb potential.

In position basis:

$$\frac{1}{2}\int v(\vec{x}_2-\vec{x}_1)\Psi^\dagger(\vec{x}_1)\Psi^\dagger(\vec{x}_2)\Psi(\vec{x}_2)\Psi(\vec{x}_1)\,\mathrm{d}^3\vec{x}_1\mathrm{d}^3\vec{x}_2.$$

It turns out that the momentum space representation is very important. Compute:

$$\begin{aligned}V_{\vec{k}_1',\vec{k}_2',\vec{k}_1,\vec{k}_2} &= \langle\vec{k}_1',\vec{k}_2'|V|\vec{k}_1,\vec{k}_2\rangle\\ &= (2\pi)^{-6}\int \exp\big(\mathrm{i}(\vec{k}_1-\vec{k}_1')\cdot\vec{x}_1+\mathrm{i}(\vec{k}_2-\vec{k}_2')\cdot\vec{x}_2\big)v(\vec{x}_2-\vec{x}_1)\,\mathrm{d}^3\vec{x}_1\mathrm{d}^3\vec{x}_2\\ &= (2\pi)^{-6}\int \exp\big(\mathrm{i}(\vec{k}_1-\vec{k}_1')\cdot\vec{x}_1+\mathrm{i}(\vec{k}_2-\vec{k}_2')\cdot\vec{x}_2\big)v(\vec{x}_2-\vec{x}_1)\,\mathrm{d}^3\vec{x}_1\mathrm{d}^3\vec{x}_2\end{aligned}$$

Now perform a (volume-preserving) change of variable to center-of-mass and relative coordinates:

$$\vec{R}=(\vec{x}_2+\vec{x}_1)/2,\qquad \vec{r}=\vec{x}_2-\vec{x}_1\quad\Leftrightarrow\quad \vec{x}_1=\vec{R}-\vec{r}/2,\qquad \vec{x}_2=\vec{R}+\vec{r}/2$$

and set

$$\vec{q}=\vec{k}_1'-\vec{k}_1.$$

Then

$$\begin{aligned}&(2\pi)^{-6}\int \exp\big(\mathrm{i}(\vec{k}_1-\vec{k}_1')\cdot\vec{x}_1+\mathrm{i}(\vec{k}_2-\vec{k}_2')\cdot\vec{x}_2\big)v(\vec{x}_2-\vec{x}_1)\,\mathrm{d}^3\vec{x}_1\mathrm{d}^3\vec{x}_2\\ =&(2\pi)^{-3}\int \exp\big(\mathrm{i}(\vec{k}_1-\vec{k}_1'+\vec{k}_2-\vec{k}_2')\vec{R}\big)\mathrm{d}^3\vec{R}\\ &(2\pi)^{-3}\int \exp\big(\mathrm{i}(\vec{k}_1'-\vec{k}_1+\vec{k}_2-\vec{k}_2')\vec{r}/2\big)v(\vec{r})\,\mathrm{d}^3\vec{r}\\ =&(2\pi)^{-3}\delta_{\vec{k}_1+\vec{k}_2,\vec{k}_1'+\vec{k}_2'}\int \exp\big(\mathrm{i}(\vec{k}_2-\vec{k}_2'-\vec{k}_1+\vec{k}_1')\vec{r}/2\big)v(\vec{r})\,\mathrm{d}^3\vec{r}\\ =&(2\pi)^{-3}\delta_{\vec{k}_1+\vec{k}_2,\vec{k}_1'+\vec{k}_2'}\int \exp\big(\mathrm{i}(\vec{k}_1'-\vec{k}_1)\vec{r}\big)v(\vec{r})\,\mathrm{d}^3\vec{r}\\ =&(2\pi)^{-3}\delta_{\vec{k}_2',\vec{k}_2-q}\tilde{v}(\vec{q}),\end{aligned}$$

in terms of the Fourier transform (up to a factors and a sign of the argument)

$$\tilde{v}(\vec{q})=\int e^{\mathrm{i}\vec{q}\cdot\vec{r}}v(\vec{r})\,\mathrm{d}^3\vec{r}.$$

So that the many-body interaction becomes

$$\frac{(2\pi)^{-3/2}}{2}\int \tilde{v}(\vec{q})a^\dagger_{\vec{k}_1+q}a^\dagger_{\vec{k}_2-q}a_{\vec{k}_2}a_{\vec{k}_1}\,\mathrm{d}^3\vec{k}_1\mathrm{d}^3\vec{k}_2\mathrm{d}^3\vec{q}$$

1.4 Bose gas

TBD.

Chapter 2

Quantization of the EM field

2.1 Electrodynamics recap

Classical electrodynamics can be described either in terms of $\vec{E}$- and $\vec{B}$-fields, or in terms of scalar and vector potential Φ, $\vec{A}$ such that

$$\vec{B} = \vec{\nabla} \times \vec{A}, \qquad \vec{E} = -\vec{\nabla}\Phi - \partial_t \vec{A}. \tag{2.1}$$

The classical Hamilton function

$$H = \frac{1}{2m}(\vec{P} - q\vec{A})^2 + q\Phi$$

for a charged particle is expressed in terms of the potential. Given the close relationship between classical Hamiltonian theory and quantum mechanics, this suggests that the potentials, rather than the fields, are the "right variables to quantize".

However, this immidiately leads to a problem: Φ, $\vec{A}$ are determined by the physical state of the EM field only up to *gauge transformations*. Recall that these are substitutions of the form

$$\vec{A} \mapsto \vec{A} + \nabla\chi, \qquad \Phi \mapsto \Phi - \partial_t \chi$$

with an arbitrary function χ. For the time being, we get rid of the ambiguity by adopting the *Coulomb gauge*, where one restricts attention to the set of vector potentials that satisfy the condition

$$\vec{\nabla} \cdot \vec{A}(t, \vec{x}) = 0. \tag{2.2}$$

We will now further restrict attention to the free-space version of Maxwell's equation, i.e. we assume that there are no charges or currents $\rho = j = 0$. In this case, the Maxwell equations become

$$\Phi(t, \vec{x}) = 0, \tag{2.3}$$

$$\left(\frac{1}{c^2}\partial_t^2 - \partial_x^2 - \partial_y^2 - \partial_z^2\right)\vec{A}(t, \vec{x}) = 0 \tag{2.4}$$

$$\vec{\nabla} \cdot \vec{A}(t, \vec{x}) = 0. \tag{2.5}$$

The space of solutions to Eq. (2.5) is spanned by plane waves of the form

$$\mathcal{A}_k \, e^{\pm i\omega_k t + i\vec{k}\vec{x}}, \qquad \omega_k := c\|\vec{k}\|$$

where we have introduced the normalization constants[1]

$$\mathcal{A}_k = \sqrt{\frac{\hbar}{2\omega_k \epsilon_0 L^3}}.$$

> At this point, we have a choice to either proceed working with complex exponentials and ensuring that imaginary parts cancel via conditions like (2.6), or else to work with a real function basis (i.e. sines and cosines), where no such conditions are necessary. Either approach has advantages and disadvantages. We go for the complex one here. Of course, this means that expressions that describe real-valued quantities (energies, field strengths, etc.) have to be such that imaginary parts cancel.

A general solution is a linear superposition of these plane waves

$$\vec{A}(t,\vec{x}) = \sum_{\vec{k}} \mathcal{A}_k \big(A^+_{\vec{k}} e^{-i\omega_k t + i\vec{k}\vec{x}} + A^-_{-\vec{k}} \, e^{+i\omega_k t - i\vec{k}\vec{x}} \big)$$

with complex expansion coeffiencts $A^{\pm}_{\vec{k}}$. The requirement that $\vec{A}(\vec{x},t)$ be real-valued is equivalent to

$$\vec{A}^-_{-\vec{k}} = \big(A^+_{\vec{k}}\big)^* \tag{2.6}$$

so that we can write the solutions as

$$\vec{A}(t,\vec{x}) = \sum_{\vec{k}} \mathcal{A}_k \, \big(\vec{A}_{\vec{k}} \, e^{-i\omega_k t + i\vec{k}\vec{x}} + \vec{A}^*_{\vec{k}} \, e^{+i\omega_k t - i\vec{k}\vec{x}} \big).$$

We have yet to incorporate the gauge condition Eq. (2.5). It reads

$$0 = \nabla \vec{A}(t,\vec{x}) = \sum_{\vec{k}} i\mathcal{A}_k \, \big(\vec{k} \cdot \vec{A}_{\vec{k}} \, e^{-i\omega_k t + i\vec{k}\vec{x}} + \vec{k} \cdot \vec{A}^*_{\vec{k}} \, e^{+i\omega_k t - i\vec{k}\vec{x}} \big).$$

Because a Fourier series is identically zero if and only if all Fourier coefficients vanish, the gauge condition is equivalent to

$$\vec{k} \cdot \vec{A}_{\vec{k}} = 0 \qquad \forall \, \vec{k} \neq 0.$$

In other words, "the Fourier coefficients $\vec{A}_{\vec{k}}$ are transversal to $\vec{k}$". We can take this into account by choosing, for each $\vec{k}$, an ortho-normal basis (the *polarization vectors*)

$$\Big\{ \vec{e}_1(\vec{k}), \vec{e}_2(\vec{k}) \Big\} \subset \{\vec{k}\}^\perp \qquad \text{with} \qquad \vec{e}_\lambda(-\vec{k}) = \vec{e}_\lambda(\vec{k})$$

for the space orthogonal to $\vec{k}$ (Fig. **??**), and setting

$$\vec{A}_{\vec{k}} = q_{\vec{k},1} \, \vec{e}_1(\vec{k}) + q_{\vec{k},2} \, \vec{e}_2(\vec{k}).$$

[1] Various conventions are in use (including a different one in earlier versions of these notes – sorry!). We follow Ref. [**?**].

In summary, applying (2.1),

$$\vec{A}(t,\vec{x}) = \sum_{\vec{k},\lambda} \mathcal{A}_k \left(q_{\vec{k}\lambda}\, \vec{e}_\lambda(\vec{k})\, e^{-i\omega_k t + i\vec{k}\vec{x}} + q^*_{\vec{k}\lambda}\, \vec{e}_\lambda(\vec{k})\, e^{+i\omega_k t - i\vec{k}\vec{x}} \right), \tag{2.7}$$

$$\vec{E}(t,\vec{x}) = i \sum_{\vec{k},\lambda} \mathcal{E}_k \left(q_{\vec{k}\lambda}\, \vec{e}_\lambda(\vec{k})\, e^{-i\omega_k t + i\vec{k}\vec{x}} - q^*_{\vec{k}\lambda}\, \vec{e}_\lambda(\vec{k})\, e^{+i\omega_k t - i\vec{k}\vec{x}} \right), \tag{2.8}$$

$$\vec{B}(t,\vec{x}) = i \sum_{\vec{k},\lambda} \mathcal{B}_k\, \vec{\kappa} \times \left(q_{\vec{k}\lambda}\, \vec{e}_\lambda(\vec{k})\, e^{-i\omega_k t + i\vec{k}\vec{x}} - q^*_{\vec{k}\lambda}\, \vec{e}_\lambda(\vec{k})\, e^{+i\omega_k t - i\vec{k}\vec{x}} \right), \tag{2.9}$$

with expansion coefficients $q_{\vec{k}\lambda} \in \mathbb{C}$ and constants

$$\mathcal{A}_k = \sqrt{\frac{\hbar}{2\omega_k \epsilon_0 L^3}}, \qquad \mathcal{E}_k = \sqrt{\frac{\hbar\omega_k}{2\epsilon_0 L^3}}, \qquad \mathcal{B}_k = \sqrt{\frac{\hbar\omega_k}{2c^2\epsilon_0 L^3}}, \qquad \vec{\kappa} = \frac{\vec{k}}{\|k\|}.$$

The plane waves indexed by a wave vector $\vec{k}$ and a polarization vector $\vec{e}_\lambda$ are called the *modes* of the EM fields.

2.2 Quick and dirty: Quantization of free fields

[$\hbar = 1$ in this section]

Here, we briefly summarize the quantization rule for *free fields*, in analogy to the harmonic oscillator. We'll give a more systematic account in terms of *canonical quantization* in the next section.

Recall the 1D harmonic oscillator, which can be treated simultaneously in a classical Hamiltonian description and in quantum Heisenberg picture. The Hamiltonian is

$$H = \frac{P^2}{2m} + \frac{m\omega^2}{2} X^2,$$

Defining

$$a = \sqrt{\frac{m\omega}{2}}(X + \frac{i}{m\omega}P), \qquad a^\dagger = \sqrt{\frac{m\omega}{2}}(X - \frac{i}{m\omega}P),$$

the Hamiltonian becomes

$$H = \omega\big(a^\dagger a + \frac{1}{2}\big).$$

Using

$$\begin{aligned} i\partial_t a(t) &= [H, a(t)] && \text{quantum commutators,} \\ \partial_t a(t) &= \{H, a(t)\} && \text{classical Poisson brackets} \end{aligned}$$

we get

$$a(t) = e^{-i\omega t} a \qquad a(t)^\dagger = e^{i\omega t} a^\dagger$$

and thus

$$X(t) = \sqrt{\frac{1}{2m\omega}}\big(ae^{-i\omega t} + a^\dagger e^{i\omega t}\big), \tag{2.10}$$

$$P(t) = i\sqrt{\frac{m\omega}{2}}\big(ae^{-i\omega t} - a^\dagger e^{i\omega t}\big). \tag{2.11}$$

There is a strong formal analogy between (2.10) and the summands in (2.7 – 2.9). A simple ansatz for a quantum theory of the EM field is thus to associate a harmonic oscillator with each mode. This turns out to give a correct description. As in the harmonic oscillator, one replaces the complex numbers $q_{\vec{k}\lambda}$ and their conjugates with Bosonic ladder operators $a_{\vec{k}\lambda}, a^*_{\vec{k}\lambda}$:

$$\hat{\vec{A}}(t,\vec{x}) = \sum_{\vec{k},\lambda} \mathcal{A}_k \left(a_{\vec{k}\lambda}\, \vec{e}_\lambda(\vec{k})\, e^{-i\omega_k t + i\vec{k}\vec{x}} + a^\dagger_{\vec{k}\lambda}\, \vec{e}_\lambda(\vec{k})\, e^{+i\omega_k t - i\vec{k}\vec{x}}\right), \tag{2.12}$$

$$\hat{\vec{E}}(t,\vec{x}) = i\sum_{\vec{k},\lambda} \mathcal{E}_k \left(a_{\vec{k}\lambda}\, \vec{e}_\lambda(\vec{k})\, e^{-i\omega_k t + i\vec{k}\vec{x}} - a^\dagger_{\vec{k}\lambda}\, \vec{e}_\lambda(\vec{k})\, e^{+i\omega_k t - i\vec{k}\vec{x}}\right), \tag{2.13}$$

$$\hat{\vec{B}}(t,\vec{x}) = i\sum_{\vec{k},\lambda} \mathcal{B}_k\, \vec{\kappa} \times \left(a_{\vec{k}\lambda}\, \vec{e}_\lambda(\vec{k})\, e^{-i\omega_k t + i\vec{k}\vec{x}} - a^\dagger_{\vec{k}\lambda}\, \vec{e}_\lambda(\vec{k})\, e^{+i\omega_k t - i\vec{k}\vec{x}}\right). \tag{2.14}$$

More explicitly: Define a single-body Hilbert space $\mathcal{H}^{(1)}$ to be the span of the mode functions $\vec{e}_{\vec{k}\lambda} e^{i\vec{k}\vec{x}}$. The Hilbert space of the EM field is taken to be the Bosonic Fock space $\mathcal{F}_S\big(\mathcal{H}^{(1)}\big)$ over the modes. As the Hamiltonian, one chooses

$$\hat{H} = \sum_{\vec{k}\lambda} \omega_k\, a^\dagger_{\vec{k}\lambda} a_{\vec{k}\lambda}$$

so that the Heisenberg picture time evolution of the ladder operators is

$$a_{\vec{k}\lambda}(t) = a_{\vec{k}\lambda} e^{-i\omega_k t}, \qquad a^\dagger_{\vec{k}\lambda}(t) = a^\dagger_{\vec{k}\lambda} e^{i\omega_k t}.$$

Equations (2.12 – 2.14) thus give the Heisenberg-pcture time evolution of observables

$$\hat{\vec{A}}(\vec{x}) = \hat{\vec{A}}(t=0,\vec{x}), \quad \hat{\vec{E}}(\vec{x}) = \hat{\vec{E}}(t=0,\vec{x}), \quad \hat{\vec{B}}(\vec{x}) = \hat{\vec{B}}(t=0,\vec{x})$$

that we postulate describe the quantized field at $\vec{x}$.

2.3 Canonical quantization

TBD: Update to more consistent normalization constants.

The "quick and dirty" quantization scheme works for non-interacting free fields and will be all you need to get through this lecture. Still, for the record, we re-derive this result using the more general *canonical quantization* procedure:

1. Choose the set of classical variables whose trajectories the theory should describe.
2. Find an action functional which is stationary exactly for the physical solutions.
3. Compute the canonical momenta and the Hamiltonian.

4. Replace each classical variable and its conjugate momentum by operators satisfying the canonical commutation relation.

5. Hope for the best! (I.e. compare predictions to experiments and re-visit any decision made if things go wrong).

In the second step, one has to express the equations of the motion (2.4) as the Euler-Lagrange equations for a suitable action functional $S[q_{\vec{k},\lambda}]$. But this is now easy! In terms of the variables $q_{\vec{k},\lambda}$, the Maxwell equations (2.4) read

$$\partial_t^2 q_{\vec{k},\lambda} + c^2 k^2 q_{\vec{k},\lambda} = 0, \tag{2.15}$$

which – for each $\vec{k}, \lambda$ – is just the equation of motion of a one-dimensional *harmonic oscillator* with angular velocity

$$\omega_{\vec{k}} = c\|\vec{k}\|.$$

Recall that the Lagrange function for such an oscillator is

$$L_{\mathrm{ho}}(q, v) = \frac{1}{2} m v^2 - \frac{1}{2} m\omega^2 q^2$$

At this point, we are free to choose m as we wish, since a global factor does not affect the set of stationary trajectories. The choice

$$m = \frac{1}{4\pi c^2} \tag{2.16}$$

will make the energy come out right later. We thus set the Lagrangian and the action functional to

$$L(q_{\vec{k},\lambda}, v_{\vec{k},\lambda}) = \frac{m}{2} \sum_{\vec{k},\lambda} \Big(\big(v_{\vec{k},\lambda}\big)^2 - \omega_k^2 \, q_{\vec{k},\lambda}^2 \Big),$$

$$S[q_{\vec{k},\lambda}] = \int L(q_{\vec{k},\lambda}(t), \dot{q}_{\vec{k},\lambda}(t)) \, \mathrm{d}t.$$

Then the Euler-Lagrange equations for stationary solutions indeed yield the Maxwell equations (2.4), so we have completed the second step of canonical quantization.

To pass to the Hamiltonian formulation compute the conjugate momenta

$$\pi_{\vec{k},\lambda} = \frac{\partial L}{\partial \dot{q}_{\vec{k},\lambda}} = m \, \dot{q}_{\vec{k},\lambda},$$

which give the Hamiltonian

$$\begin{aligned} H(q_{\vec{k},\lambda}, \pi_{\vec{k},\lambda}) &= \sum_{\vec{k},\lambda} m \dot{q}_{\vec{k},\lambda} \pi_{\vec{k},\lambda} - L \\ &= \sum_{\vec{k},\lambda} \left(\frac{1}{2m} \pi_{\vec{k},\lambda}^2 + \frac{1}{2} m\omega_k^2 \, q_{\vec{k},\lambda}^2 \right) \\ &= \sum_{\vec{k},\lambda} \Big(\frac{1}{4m} (\pi_{\vec{k},\lambda}^2 + \pi_{-\vec{k},\lambda}^2) + \frac{1}{4} m\omega_k^2 (q_{\vec{k},\lambda}^2 + q_{-\vec{k},\lambda}^2) \Big) \\ &= \sum_{\vec{k},\lambda} \Big(\frac{1}{2m} \pi_{\vec{k},\lambda} \pi_{-\vec{k},\lambda} + \frac{1}{2} m\omega_k^2 q_{\vec{k},\lambda} q_{-\vec{k},\lambda} \Big). \end{aligned}$$

We will use the final expression, as it is manifestly real-valued and non-negative under the constraints (2.6).

On to the final step of quantization! We would like to have operators $\hat{q}_{\vec{k}\lambda}$ and $\hat{\pi}_{\vec{k}\lambda}$ that fullfil the canonical commutation relations

$$[\hat{q}_{\vec{k}\lambda}, \hat{\pi}_{\vec{k}'\lambda'}] = \mathrm{i}\hbar\delta_{\vec{k}\lambda,\vec{k}'\lambda'}, \qquad [\hat{q}_{\vec{k}\lambda}, \hat{q}_{\vec{k}'\lambda'}] = 0, \qquad [\hat{\pi}_{\vec{k}\lambda}, \hat{\pi}_{\vec{k}'\lambda'}] = 0. \tag{2.17}$$

In the quantum mechanical description of a point particle, the position and momentum observables describe real values, and are thus chosen to be Hermitian. As a result of our choice to work with complex exponentials, the $q_{\vec{k}\lambda}$'s and $\pi_{\vec{k}\lambda}$'s are complex, but satisfy $q_{-\vec{k},\lambda} = q^*_{\vec{k},\lambda}, \pi_{-\vec{k},\lambda} = \pi^*_{\vec{k},\lambda}$. In order to reproduce this behavior in the quantum theory, we will look for operators that satisfy

$$\hat{q}_{-\vec{k},\lambda} = \hat{q}^\dagger_{\vec{k},\lambda}, \qquad \hat{\pi}_{-\vec{k},\lambda} = \hat{\pi}^\dagger_{\vec{k},\lambda}. \tag{2.18}$$

Let's construct a concrete realization of such operators. To this end, we start with the space of all vector potentials $\vec{A}(\vec{x})$ that satisfy the gauge condition (2.5), allow for complex linear combinations, and interpret it as a single-body Hilbert space $\mathcal{H}^{(1)}$ with the usual inner product on function spaces. Using our analysis, we can take

$$\mathcal{H}^{(1)} = L^2(R) \otimes \mathbb{C}^2, \tag{2.19}$$

with momentum basis $\{|\vec{k}, \lambda\rangle\}_{\vec{k},\lambda}$. Here, R is the region in space (i.e. the box of extension $L \times L \times L$) we are considering. On the symmetric Fock space

$$\mathcal{H}_{EM} := \mathcal{F}_S\big(\mathcal{H}^{(1)}\big),$$

there are the now-familiar creation operators $a^\dagger_{\vec{k}\lambda}$ that fulfill

$$[a_{\vec{k}\lambda}, a^\dagger_{\vec{k}'\lambda'}] = \delta_{\vec{k}\lambda,\vec{k}'\lambda'}, \qquad [a^\dagger_{\vec{k}\lambda}, a^\dagger_{\vec{k}'\lambda'}] = 0, \qquad [a_{\vec{k}\lambda}, a_{\vec{k}'\lambda'}] = 0. \tag{2.20}$$

Then the choice

$$\hat{q}_{\vec{k}\lambda} = \sqrt{\frac{\hbar}{2m\omega_k}}\big(a^\dagger_{-\vec{k}\lambda} + a_{\vec{k}\lambda}\big), \qquad \hat{\pi}_{\vec{k}\lambda} = \mathrm{i}\sqrt{\frac{\hbar m\omega_k}{2}}\big(-a^\dagger_{-\vec{k}\lambda} + a_{\vec{k}\lambda}\big)$$

gives a solution to (2.17) and (2.18):

$$[\hat{q}_{\vec{k}\lambda}, \hat{\pi}_{\vec{k}'\lambda'}] = \delta_{\vec{k}\lambda,\vec{k}'\lambda'}\frac{\mathrm{i}\hbar}{2}\big(-[a^\dagger_{-\vec{k}\lambda}, a_{-\lambda k}] + [a_{\vec{k}\lambda}, a^\dagger_{\vec{k}\lambda}]\big) = \mathrm{i}\hbar\delta_{\vec{k}\lambda,\vec{k}'\lambda'}.$$

We now substitute $q_{\vec{k}\lambda} \to \hat{q}_{\vec{k}\lambda}$, $\pi_{\vec{k}\lambda} \to \hat{\pi}_{\vec{k}\lambda}$ to get candidate quantum expressions for observables. In particular, the Hamiltonian reads

$$\begin{aligned}
\hat{H} &= \sum_{\vec{k},\lambda}\Big(\frac{1}{2m}\hat{\pi}_{\vec{k},\lambda}\hat{\pi}_{-\vec{k},\lambda} + \frac{1}{2}m\omega_k^2\hat{q}_{\vec{k},\lambda}\hat{q}_{-\vec{k},\lambda}\Big) \\
&= \sum_{\vec{k},\lambda}\Big(-\frac{\hbar\omega_k}{4}(a^\dagger_{\vec{k}\lambda} - a_{-\vec{k}\lambda})(a^\dagger_{-\vec{k}\lambda} - a_{\vec{k}\lambda}) + \frac{\hbar\omega_k}{4}(a^\dagger_{-\vec{k}\lambda} + a_{\vec{k}\lambda})(a^\dagger_{\vec{k}\lambda} + a_{-\vec{k}\lambda})\Big) \\
&= \sum_{\vec{k},\lambda}\hbar\omega_k\Big(a^\dagger_{\vec{k}\lambda}a_{\vec{k}\lambda} + \frac{1}{2}\Big),
\end{aligned} \tag{2.21}$$

which is just the Hamiltonian of one harmonic oscillator per choice of $\vec{k}, \lambda$. We got ourselves a candidate quantum theory of the electro-magnetic field! Now let's check whether it produces reasonable results.

When we apply (2.21) to the vaccum state, we get

$$\hat{H}|\text{vac}\rangle = \sum_{\vec{k},\lambda} \frac{1}{2} c\hbar \|\vec{k}\| |\,\text{vac}\rangle,$$

which diverges. What to make of this? One could just "renormalize" the Hamiltonian in (2.21), by substracting $1/2$ from each term. This seems innocent enough, as only energy *differences* cause observable effects in quantum theory. However, there are reasons to worry about such a step. In general relativity, energy gives rise to gravitation, so there the absolut scale *does* matter. If we want to (and we do!) build a theory of quantum gravity, we shouldn't be so cavalier about throwing out contributions that the theory naturally gives to us. There is also a semi-classical calculation of the *Casimir effect* – an attractive force between two parallel conductors – that relies on the "zero point energy term" $1/2\hbar\omega_k$ and seems to give right results. Neither argument *proves* that the term should be there (because we don't know what a successful quantum theory of gravity will look like, and because Casimir's calculation does not treat the conductors quantum mechanically, as one really should), but they suggest we be cautious. Another way to rid ourselves of the divergences would be to truncate the sum, by introducing a "cut-off" condition $\|\vec{k}\| < K$ for some large K (the Casimir calculation involves such a cut-off). This could be justified if we assume that existing theories cease to be accurate at high energies and must be replaced by a more general, as of yet unknown, description. Trouble is, despite the esthetic draw-back of the odd infinity cropping up in calculations, the predictions made by the quantum theory of light work etremely well in practice, so there is little guidance as to how a more general framework might look like. So, really, there is no good answer, presently, for how to think about this and other infinities.

In the last chapter, we started with a single-body Hilbert space $\mathcal{H}^{(1)}$ and passed to Fock space over it, in order to describe many-body states. In the quantum theory of light, similar objects appear, but the logic is reversed! The quantization process directly gives rise to a Fock space. The single-body space $\mathcal{H}^{(1)}$ that appears in (2.19) is just an auxilliary tool. We have not associated a quantum theory with $\mathcal{H}^{(1)}$. Some researchers have tried to interpret $\mathcal{H}^{(1)}$ as a space of "wave functions for a single photon", but it is unclear whether this is a helpful approach. We will come back to this point when we look at relativistic quantum mechanics...

Like the Hamiltonian, we can now associate observables with other physical quantities.

The vector potential in position basis:

$$\begin{aligned}
\hat{\vec{A}}(\vec{x}) &= \frac{1}{\sqrt{L^3}} \sum_{\vec{k},\lambda} \hat{q}_{\vec{k}\lambda} e^{i\vec{k}\cdot\vec{x}}\, \vec{e}_\lambda(\vec{k}) \\
&= \sum_{\vec{k},\lambda} \sqrt{\frac{\hbar}{2m\omega_k L^3}} (a^\dagger_{-\vec{k}\lambda} + a_{\vec{k}\lambda}) e^{i\vec{k}\cdot\vec{x}}\, \vec{e}_\lambda(\vec{k}) \\
&= \sqrt{\frac{2\pi\hbar c^2}{L^3}} \sum_{\vec{k},\lambda} \frac{\vec{e}_\lambda(\vec{k})}{\sqrt{\omega_k}} (a^\dagger_{\vec{k}\lambda} e^{-i\vec{k}\cdot\vec{x}} + a_{\vec{k}\lambda} e^{i\vec{k}\cdot\vec{x}}),
\end{aligned}$$

having re-arranged summands in the last step.

For the field operators, classically,

$$\vec{E}(\vec{x},t) = -\frac{1}{c}\partial_t \vec{A}(\vec{x},t) = -\frac{1}{c\sqrt{L^3}}\sum_{\vec{k},\lambda} \dot{q}_{\vec{k}\lambda} e^{i\vec{k}\vec{x}}\,\vec{e}_\lambda(\vec{k}) = -\frac{1}{mc\sqrt{L^3}}\sum_{\vec{k},\lambda} \pi_{\vec{k}\lambda} e^{i\vec{k}\vec{x}}\,\vec{e}_\lambda(\vec{k})$$

$$\vec{B}(\vec{x},t) = \vec{\nabla}\times\vec{A}(\vec{x},t) = \frac{1}{\sqrt{L^3}}\sum_{\vec{k},\lambda}\vec{\nabla}\times\left(q_{\vec{k}\lambda}e^{i\vec{k}\vec{x}}\,\vec{e}_\lambda(\vec{k})\right) = \frac{1}{\sqrt{L^3}}\sum_{\vec{k},\lambda} i\vec{k}\times\left(q_{\vec{k}\lambda}e^{i\vec{k}\vec{x}}\,\vec{e}_\lambda(\vec{k})\right)$$

so that the operators become

$$\hat{\vec{E}}(\vec{x}) = -i\sqrt{\frac{2\pi\hbar}{L^3}}\sum_{\vec{k},\lambda}\sqrt{\omega_k}\,\vec{e}_\lambda(\vec{k})\,(a^\dagger_{\vec{k}\lambda}e^{-i\vec{k}\vec{x}} - a_{\vec{k}\lambda}e^{i\vec{k}\vec{x}}),$$

$$\hat{\vec{B}}(\vec{x}) = i\sqrt{\frac{2\pi\hbar c^2}{L^3}}\sum_{\vec{k},\lambda}\frac{\vec{k}\times\vec{e}_\lambda(\vec{k})}{\sqrt{\omega_k}}(a^\dagger_{\vec{k}\lambda}e^{-i\vec{k}\vec{x}} - a_{\vec{k}\lambda}e^{i\vec{k}\vec{x}}).$$

Field commutator: Because the field $\vec{E}(\vec{x})$ is expressed in terms of the conjugate momenta $\pi_{\vec{k}\lambda}$, while $\vec{B}(\vec{x})$ is a function of the $q_{\vec{k}\lambda}$, the associated operators do not commute. A lengthy calculation gives

$$[\hat{E}_x(\vec{x}), \hat{B}_y(\vec{x}')] = i4\pi\hbar\partial_z\delta(\vec{x}-\vec{x}')$$

and expressions resulting from a cyclic permutations of the coordinates. This means that the E and B field at the same point are *not* simultaneously well-defined.

Time evolution: It is often useful to describe the time evolution of the field operators in Heisenberg picture:

$$\hat{\vec{E}}(\vec{x},t) := e^{-\frac{t}{i\hbar}\hat{H}}\,\hat{\vec{E}}(\vec{x})\,e^{\frac{t}{i\hbar}\hat{H}}$$

which solves the Heisenberg picture Schrödinger equation

$$-i\hbar\partial_t\,\hat{\vec{E}}(\vec{x},t) = [H, \hat{\vec{E}}(\vec{x},t)].$$

This works exactly as in the case of the position and momentum operators for a simple harmonic oscillator. It suffices to verify that

$$a^\dagger_k(t) = a^\dagger_k e^{i\omega_k t} \qquad \text{and thus} \qquad a_k(t) = a_k e^{-i\omega_k t}$$

are the right expressions for the Heisenberg-picture ladder operators. Thus

$$\begin{aligned}\hat{\vec{E}}(\vec{x},t) &= -i\sqrt{\frac{2\pi\hbar}{L^3}}\sum_{\vec{k},\lambda}\sqrt{\omega_k}\,\vec{e}_\lambda(\vec{k})\,(a^\dagger_{\vec{k}\lambda}(t)e^{-i\vec{k}\vec{x}} - a_{\vec{k}\lambda}(t)e^{i\vec{k}\vec{x}})\\ &= -i\sqrt{\frac{2\pi\hbar}{L^3}}\sum_{\vec{k},\lambda}\sqrt{\omega_k}\,\vec{e}_\lambda(\vec{k})\,(a^\dagger_{\vec{k}\lambda}e^{-i\vec{k}\vec{x}+i\omega_k t} - a_{\vec{k}\lambda}e^{i\vec{k}\vec{x}-i\omega_k t}).\end{aligned}$$

2.4 States of the EM field

2.4.1 Number states

Let enumerate all modes $(\vec{k}, \lambda)$ of the EM field by natural numbers $k \in \mathbb{N}$ in some way. Then one can define an occuptation number basis

$$|n_1, \dots\rangle$$

for the field, where n_k gives the number of excitations (photons) in mode $\vec{k}_k, \lambda_k$. Elements of the occupation number basis – i.e. states with a definite number of photons in each mode – are called *number states* or *Fock states*. The single most important Fock state is the vaccum $|\text{vac}\rangle$ with zero occupancy in every mode.

The *expected* electric field strength in any number state is

$$\langle n_1 \dots |\vec{E}(\vec{x})|n_1 \dots\rangle \propto \sum_k \langle n_1 \dots |\vec{e}_k(a_k^\dagger e^{-i\vec{k}\vec{x}} - a_k e^{i\vec{k}\vec{x}})|n_1 \dots\rangle = 0.$$

(That's the same kind of calcualtion that show that eigenstates of the harmonic oscillator have vanishing position and momentum expectations). Zero fields on average does not imply zero fields all the time. Let's compute the expected absolut value squared of the field

$$\begin{aligned}
&\langle n_1 \dots |\vec{E}(\vec{x}) \cdot \vec{E}(\vec{x})|n_1 \dots\rangle \\
&= -\frac{2\pi\hbar}{L^3} \sum_{k,k'} \sqrt{\omega_k \omega_{k'}} \big(\vec{e}_k \cdot \vec{e}_k\big) \langle n_1 \dots |\big(a_k^\dagger e^{-i\vec{k}\vec{x}} + a_k e^{i\vec{k}\vec{x}}\big)\big(a_k^\dagger e^{-i\vec{k}'\vec{x}} + a_k e^{i\vec{k}'\vec{x}}\big)|n_1 \dots\rangle
\end{aligned}$$

(only cross terms involving the same k survive)

$$\begin{aligned}
&= \frac{2\pi\hbar}{L^3} \sum_k \omega_k \langle n_1 \dots |a_k^\dagger e^{-i\vec{k}\vec{x}} a_k e^{i\vec{k}\vec{x}} + a_k e^{-i\vec{k}\vec{x}} a_k^\dagger e^{i\vec{k}\vec{x}}|n_1 \dots\rangle \\
&= \frac{4\pi\hbar}{L^3} \sum_k \omega_k (n_k + 1/2) \to \infty.
\end{aligned}$$

Another infinity! This one can't be dismissed by substracting the $1/2$ as we did for the energies. Outside of GR, only energy differences have observable effects – but the field strength is directly proportional to the force exerted on a charged body. The occurance of high field strengths (in random directions) even for the vaccum state are the infamous *vaccuum fluctuations*. Should we be worried that all charged particles in our bodies will be catapulted into orbit by a vacuum fluctuation of the electric field any time?

It turns out that this particular infinity can easily be tamed. Field strength is measured via the force on a charged particle. Realistically, these particles have finite extend, so cannot be concentrated on just one point $\vec{x}$ in space. If we replace the point-sized probe by one with a charge density $\rho(\vec{x})$, then one can show (excercise!) that the spatially averaged force

$$\vec{F} := \int \rho(\vec{x}) \vec{E}(\vec{x}) \, \mathrm{d}^3\vec{x}$$

has finite fluctuations, if ρ is sufficiently spread out. This is physically plausible. The divergence was caused by terms with large wave vector $\vec{k}$. But these correspond to

fields that will oscillate rapidly, so that cancellations over any finite region will cause the net force to be small.

> Interestingly, the concept of point charges already causes headaches in classical electrodynamics: The energy contained in the electric field of a point charge is infinite. So, really, smear out your chages to avoid trouble!

2.4.2 Coherent states

You may remember the *coherent states* of a single harmonnic oscillator from your quantum mechanics lecture. For $\alpha \in \mathbb{C}$, these are defined as

$$|\alpha\rangle = e^{-|\alpha|^2/2} \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}} |n\rangle.$$

Coherent states are eigenvectors of the annihilation operator

$$\begin{aligned} a|\alpha\rangle &= e^{-|\alpha|^2/2} \sum_{n=1}^{\infty} \frac{\alpha^n}{\sqrt{n!}} \sqrt{n} |n-1\rangle \\ &= e^{-|\alpha|^2/2} \sum_{n'=0}^{\infty} \frac{\alpha^{n'+1}}{\sqrt{(n'+1)!}} \sqrt{n'+1} |n'\rangle \\ &= \alpha\, |\alpha\rangle. \end{aligned}$$

A coherent state $|\alpha_1, \ldots\rangle$ of the entire EM field is one where each mode $k \equiv (\vec{k}, \lambda)$ is in a coherent state $|\alpha_k\rangle$.

2.5 Light-matter interaction

Recall the Hamiltonian of a single electron in a magnetic field

$$\hat{H} = \frac{\left(\hat{\vec{P}} - \frac{e}{c}\hat{\vec{A}}\right)^2}{2m} + \hat{V}$$

(we neglect any spin degrees of freedom for now). In the introductory QM class, the vector potential was treated "classically", i.e. as a multiplication operator by the classical field

$$\hat{\vec{A}} |\vec{r}\rangle = \vec{A}(\vec{r}) |\vec{r}\rangle$$

acting only on electron Hilbert space $\mathcal{H}_e = L^2(\mathbb{R}^3)$.

We will now work with the joint system, comprised of a single electron and the quantized EM field. The joint Hilbert space is $\mathcal{H}_e \otimes \mathcal{H}_{EM}$. Both the set of possible positions of the electron, and the set of positions where one can measure the fields are labeled by vectors in $\mathbb{R}^3$. To keep them apart, we'll use $\vec{r}$ for the labels of the position basis of the electron, and $\vec{x}$ for the labels of the field operators. For example:

$$\left(\hat{\vec{R}} \otimes \hat{\vec{A}}(\vec{x})\right) |\vec{r}\rangle_e \otimes |n_1 \ldots\rangle_{EM} = \left(\vec{r}|\vec{r}\rangle_e\right) \otimes \left(\hat{\vec{A}}(\vec{x}) |n_1 \ldots\rangle_{EM}\right)$$

However, one can also *couple* the two systems, e.g. by evaluating the field operator at the position of the electron

$$\big(\hat{\vec{A}}(\hat{\vec{R}})\big)\,|\vec{r}\rangle_e \otimes |n_1 \dots\rangle_{EM} = \big(|\vec{r}\rangle_e\big) \otimes \big(\hat{\vec{A}}(\vec{r})|n_1 \dots\rangle_{EM}\big).$$

If you like analysis, just write $\hat{\vec{A}}(\vec{r})$, calculate away, and everything will work. If you like linear algebra, then the expression

$$\hat{\vec{A}}(\hat{\vec{R}}) = \int |\vec{r}\rangle\langle\vec{r}| \otimes \hat{\vec{A}}(\vec{r})\,\mathrm{d}^3\vec{r}$$

might be helpful.

In any case, the Hamiltonian

$$\hat{H} = \frac{\big(\hat{\vec{P}} - \frac{e}{c}\hat{\vec{A}}(\hat{\vec{R}})\big)^2}{2m} + \hat{V} - 2\mu_B \hat{\vec{S}} \cdot \hat{\vec{B}}(\hat{\vec{R}}), + \sum_k \hbar\omega_k a_k^\dagger a_k$$

describes a single electron coupled to the quantized EM field. To describe multiple electrons, pass to the many-body picture also for the matter part

$$\hat{H} = \sum_{ij} \left\langle \phi_i \right| \frac{\big(\hat{\vec{P}} - \frac{e}{c}\hat{\vec{A}}(\hat{\vec{R}})\big)^2}{2m} + \hat{V} - 2\mu_B \hat{\vec{S}} \cdot \hat{\vec{B}}(\hat{\vec{R}}) \left| \phi_j \right\rangle b_i^\dagger b_j + \sum_k \hbar\omega_k a_k^\dagger a_k$$

for some single-body basis $\{\phi_i\}_i$.

As you could have guessed, we'll need to resort to approximations and to perturbation theory to make progress. For now, we'll

- Neglect the magnetic field $\vec{B}$ and two-photon processes $(\vec{A})^2$.

Next, realize that in Coulomb gauge, the momentum operator and the vector potential commute.

$$\begin{aligned}\Big(\vec{\nabla}_{\vec{r}}\hat{\vec{A}}(\hat{\vec{R}})\psi\Big)(\vec{r}; s; n_1 \dots) &= \vec{\nabla}_{\vec{r}}\Big(\hat{\vec{A}}(\vec{r})\psi(\vec{r}; s; n_1 \dots)\Big) \\ &= \Big(\vec{\nabla}_{\vec{r}}\hat{\vec{A}}(\vec{r})\Big)\psi(\vec{r}; s; n_1 \dots) + \hat{\vec{A}}(\vec{r})\vec{\nabla}_{\vec{r}}\psi(\vec{r}; s; n_1 \dots) \\ &= \hat{\vec{A}}(\vec{r})\vec{\nabla}_{\vec{r}}\psi(\vec{r}; s; n_1 \dots).\end{aligned}$$

Thus, the approximate Hamiltonian becomes

$$\hat{H} = \hat{H}_0 + \hat{H}_I \qquad H_0 = \frac{\hat{\vec{P}}^2}{2m} + \hat{V} + \sum_k \hbar\omega_k a_k^\dagger a_k, \qquad H_I = -\frac{e}{cm}\hat{\vec{A}} \cdot \hat{\vec{P}}.$$

TBD

Express interaction Hamiltonian in many-body picture w.r.t. an atomic set of basis

functions $\{\phi_i\}$.

$$\begin{aligned}
&-\sum_{ij}\langle\phi_i|H_I|\phi_j\rangle b_i^\dagger b_j \\
=&-\frac{e}{cm}\sum_{ij}\langle\phi_i|\hat{\vec{P}}\cdot\hat{\vec{A}}|\phi_j\rangle b_i^\dagger b_j \\
=&-\frac{e}{m}\sqrt{\frac{2\pi\hbar c^2}{L^3}}\sum_{ijk}\int\phi_i^*(\vec{x})\frac{1}{\sqrt{\omega_k}}(a_k^\dagger e^{-i\vec{k}\vec{x}}+a_k e^{i\vec{k}\vec{x}})\vec{e}_k\cdot\hat{\vec{P}}\phi_j(\vec{x})\,\mathrm{d}^3\vec{x}\,b_i^\dagger b_j \\
=&-\frac{e}{m}\sqrt{\frac{2\pi\hbar c^2}{L^3}}\sum_{ijk}\int\phi_i^*(\vec{x})\frac{1}{\sqrt{\omega_k}}((a_k^\dagger+a_{-k})e^{-i\vec{k}\vec{x}})\vec{e}_k\cdot\hat{\vec{P}}\phi_j(\vec{x})\,\mathrm{d}^3\vec{x}\,b_i^\dagger b_j \\
=&-\sum_{ijk}g_{ijk}(a_k^\dagger+a_{-k})b_i^\dagger b_j
\end{aligned}$$

with coupling constants

$$g_{ijk}=-\frac{e}{m}\sqrt{\frac{2\pi\hbar c^2}{L^3}}\frac{1}{\sqrt{\omega_k}}\int\phi_i^*(\vec{x})e^{-i\vec{k}\vec{x}}\vec{e}_k\cdot\hat{\vec{P}}\phi_j(\vec{x})\,\mathrm{d}^3\vec{x}.$$

in dipole approximation

$$g_{ijk}\simeq-\frac{e}{m}\sqrt{\frac{2\pi\hbar c^2}{L^3}}\frac{1}{\sqrt{\omega_k}}\int\phi_i^*(\vec{x})\vec{e}_k\cdot\hat{\vec{P}}\phi_j(\vec{x})\,\mathrm{d}^3\vec{x}.$$

Trick:

$$[\hat{\vec{R}},\hat{H}_0]=\frac{i\hbar}{m}\hat{\vec{P}},\qquad\Rightarrow\qquad\hat{\vec{P}}=\frac{m}{i\hbar}[\hat{\vec{R}},H_0].$$

The coupling constants become

$$\begin{aligned}
g_{ijk}&=-\frac{e}{m}\sqrt{\frac{2\pi\hbar c^2}{L^3}}\frac{1}{\sqrt{\omega_k}}\langle\phi_i|(\vec{e}_k\cdot\hat{\vec{P}})|\phi_j\rangle \\
&=i\sqrt{\frac{2\pi e^2c^2}{\hbar L^3}}\frac{1}{\sqrt{\omega_k}}(E_j-E_i)\langle\phi_i|(\vec{e}_k\cdot\hat{\vec{R}})|\phi_j\rangle.
\end{aligned}$$

Because this expression is symmetric under inversion of $\vec{k}$, the annoying minus sign in the field-atom Hamiltonian can be dropped

$$\sum_{ij}\langle\phi_i|H_I|\phi_j\rangle b_i^\dagger b_j=\sum_{ijk}g_{ijk}(a_k^\dagger+a_k)b_i^\dagger b_j\qquad\text{under dipole approximation.}$$

2.5.1 Emission and Absorption

We now apply Fermi's Golden Rule to the field-atom Hamiltonian. The unperturbed states are labelled by a set of occupied atomic orbitals and a list of occupation numbers for the field. Let's assume that there's only one electron. Then, to apply FGR, we have to compute the matrix elements (in Dipole approximation)

TBD

Chapter 3

Relativistic QM

[In this chapter, we set $\hbar = c = 1$.]

The first thing to know about relativistic QM is that it doesn't really work. The initial goal was to find a relativistc replacement for the Schrödinger equation

$$\big(i\partial_t - \frac{1}{2m}\sum_{i=1}^{3}\partial_{x_i}^2\big)\psi = 0$$

that treats temporal and spatial coordinates radically differently. Two Lorentz-invariant wave equations emerged as candidates: The Klein-Gordon and the Dirac equation. Attempts to interpret their solutions as wave functions for a single particle failed for a number of reasons – e.g. the emergence of states of unbounded negative energy, and the absence of a conserved quantity that could be interpreted as a probability. But the results were not in vain. One can re-interpret the solutions as a single-particle Hilbert space, then construct a Fock space over it, and thus obtain a quantum field theory. The resulting relativistic quantum field theories are no longer plagued by the mentioned inconsistencies (negative energies, no probabilities). And although new problems appear, they turn out to be hugely successful and form the basis of high-energy physics. The process is strongly analogous to the quantizatin of the EM field, with the Klein-Gordon or, respectively, the Dirac equation taking the place of the Maxwell equation.

With the benefit of hindsight, one could now directly introduce relativistic QFT, without taking the ultimately unsuccessful detour of constructing a single-particle theory. This is done, e.g. in Ref. [**?**]. While such a presentation has a more straight-forward logic, the disadvantage is that it takes a considerable amount of technical preparation before first results can be achieved. Lacking the time, we will take the historic route here.

3.1 Special Relativity recap

Recall the basic assumptions of special relativity: 1) All inertial frames are equivalent, and 2) the speed of light is constant in any interntial frame. The second axiom implies that velocities can no longer be linearly added as is true in Galilean space-time. Instead, when transforming into a reference frame that travels with a constant relative velocity (along, say, the x-axis), one has to employ a *Lorentz boost* that mixes space- and time

variables:

$$t' = \gamma(t + \beta x), \quad x' = \gamma(\beta t + x), \quad y' = y, \quad z' = z, \qquad \gamma = \frac{1}{\sqrt{1+\beta^2}},$$

where β is the velocity in units of c.

It turns out that these axioms imply that space-time should be though of as $\mathbb{R}^4$ with *Minkowski inner product*

$$\langle x, y\rangle = (x, gy), \qquad g = \begin{pmatrix} 1 & & & \\ & -1 & & \\ & & -1 & \\ & & & -1 \end{pmatrix}. \tag{3.1}$$

The *(homogenous) Lorentz group* $O(1,3)$ is the set of 4×4 matrices Λ that leave (3.1) invariant

$$\langle \Lambda x, \Lambda y\rangle = \langle x, y\rangle.$$

Because

$$\langle \Lambda x, \Lambda y\rangle = (x, \Lambda^t g \Lambda y)$$

the Lorentz group can be expressed as

$$O(1,3) = \{\Lambda \mid \Lambda^t g \Lambda = g\}.$$

The *Poincaré group*, or *inhomogeneous Lorentz group* is the set of affine transformations

$$x \mapsto x' = \Lambda x + a, \qquad \Lambda \in O(1,3), a \in \mathbb{R}^4.$$

These are exactly the transformations between inertial frames. The Poincaré group is thus the relativistic analogue of the Galileo group. We will study these groups in much more detail below.

When we say that a theory is "relativistic", we mean that the its predictions are the same for any pair of observers that is related by a Poincaré transformation. In order to construct relativistic theories, we will therefore have to investigate how the description of various geometric objects changes when passing between inertial reference frames. This is up next, first focussing on the Lorentz group.

3.1.1 Coordinate transformations on space-time

We will introduce some important objects on space-time $\mathbb{R}^4$, first in a coordinate-free way, and then in coordinates. Everyone should understand at least one of the two approaches.

Coordinate-free approach

Consider two reference frames that are connected by a Lorentz transformation Λ (Fig. **??**). In other words, if some event has space-time coordinates $x \in \mathbb{R}^4$ in the first reference frame, its coordinates in the second one are

$$x' = \Lambda x. \tag{3.2}$$

The relation (3.2) is called *contravariant transformation law*.

Elements of $\mathbb{R}^4$ may describe other types of objects, not just space-time coordinates. For example, consider a plane wave

$$\phi(x) = \cos\big((p,x)\big)$$

whose phase is given by a linear function

$$x \mapsto (p,x) = \sum_{i=1}^{4} p_i x_i$$

which is expressed as a *Euclidean* inner product (also called a *contraction* in this context). Since the phase is a physical property of the wave that does not depend on the coordinates used to describe it, we must have $(p,x) = (p',x')$. Because

$$(p',x') = (p',\Lambda x) = (\Lambda^t p', x)$$

this is equivalent to

$$p' = \big(\Lambda^t\big)^{-1} p =: \Lambda^{-t} p. \tag{3.3}$$

Relation (3.3) is called the *covariant transformation law*. (Linear functionals are also called *co*vectors, so the name makes sense). In general, the contraction (p,x) between any covariant p and contravariant x is *invariant*.

Another important object that follows a covariant transformation law is the *gradient*. By the chain rule,

$$\nabla_i = \frac{\partial}{\partial x_i} = \sum_j \frac{\partial x'_j}{\partial x_i}\,\frac{\partial}{\partial x'_j} = \sum_j \frac{\partial(\Lambda x)_j}{\partial x_i}\,\frac{\partial}{\partial x'_j} = \sum_j \Lambda^j{}_i\,\frac{\partial}{\partial x'_j} = \big(\Lambda^t \nabla'\big)_i$$

and hence

$$\nabla' = \Lambda^{-t}\nabla.$$

With every vector x, one can associate the functional

$$y \mapsto \langle y, x\rangle = (y, gx),$$

i.e. the "Minkowski projetion onto x". (This is similar to turning a *ket* into a *bra* in QM – just that in this case, the operation is linear rather than anti-linear). From the above discussion of the transformation laws of functionals, it follows that gx is covariant. There's another way of seeing this: From the definition of the Lorentz group,

$$\Lambda^t g \Lambda = g \quad \Rightarrow \quad g\Lambda = \Lambda^{-t} g$$

and thus, under a Lorentz transformation,

$$gx \mapsto g\Lambda x = \Lambda^{-t} g x.$$

Finally, let's look at the transformation behavior of functions and fields. Let $\phi : \mathbb{R}^4 \to \mathbb{R}$ be a scalar function whose value at a point x has a direct physical interpration

and can thus not depend on the coordinates (e.g. the phase of the plane wave above, or, say, the pressure of a fluid). Then

$$\phi'(x') = \phi(x) = \phi(\Lambda^{-1}x').$$

In other words,

$$\phi' = \phi \circ \Lambda^{-1}.$$

Mind the inverse! The transformation law of vector-valued functions, or *vector fields*, $F : \mathbb{R}^4 \to \mathbb{R}^m$ depends on the geometric interpretation of the vector $F(x)$ at a point. Take the *gradient field*

$$F(x) = \nabla f(x)$$

of some scalar function f as an example. Combining what we already know:

$$F'(x') = \Lambda^{-t} F(\Lambda^{-1}x').$$

This is one instance of the more general rule

$$F'(x') = D(\Lambda)F(\Lambda^{-1}x'), \tag{3.4}$$

for some $m \times m$-matrix $D(\Lambda)$ which depends on the geometric interpretation of the field. We'll encounter quite non-trivial behavior!

Ricci calculus

For calculations, we'll use the *Ricci calculus* or *covariant notation*. It's based on the following conventions: Write x^μ to refer either to

- the μ-th component of a contravariant vector $x \in \mathbb{R}^4$ (here, we think of μ as a *specific* number from $\{0, 1, 2, 3\}$); or
- the entire vector $x \in \mathbb{R}^4$ (thinking of μ is a variable).

This constructive ambiguity might seem confusing, but it works well in practice. (In fact, you are already familiar with similar conventions. E.g. the notation $f(x)$ might refer to the value of a function f at some specific x, or to the rule $f : x \mapsto f(x)$ in its entirety). More generally, we'll use this dictionary:

contravariant vector	x	x^μ
covariant vector	p	p_μ
linear map (matrix)	M	$M^\mu{}_\nu$
metric	g	$g_{\mu\nu}$,
inverse metric	g^{-1}	$g^{\mu\nu}$,

where $M^\mu{}_\nu, g_{\mu\nu}$, and $g^{\mu\nu}$ are the matrix elements of M, g, and g^{-1} respectively. (In our case, $g = g^{-1}$, but keep the distinction, as the calculus also work with more general metrics). Next, we employ the *Einstein summation convention* which states that indices that appear repeatedly in a product are summed over. Then the standard operations of

linear algebra take the following form:

matrix-vector multiplication	$y = Mx$	$y^\mu = M^\mu{}_\nu x^\nu$
lowering index	gx	$x_\mu = g_{\mu\nu}x^\nu$
raising index	$g^{-1}p$	$p^\mu = g^{\mu\nu}p_\nu$
Minkowski inner product	$\langle x, y\rangle = (x, gy)$	$x^\mu g_{\mu\nu} y^\nu = x^\mu y_\nu = x_\mu y^\nu$
contraction	(p, x)	$p_\mu x^\mu$
inverse-transpose Lorentz trans.	$\Lambda^{-t} = g\Lambda g^{-1}$	$g_{\mu\alpha}\Lambda^\alpha{}_\beta g^{\beta\nu} = \Lambda_\mu{}^\nu$
contravariant transformation	$\tilde{x} = \Lambda x$	$\tilde{x}^\mu = \Lambda^\mu{}_\nu x^\nu$
covariant transformation	$\tilde{p} = \Lambda^{-t} p$	$\tilde{p}_\mu = \Lambda_\mu{}^\nu p_\nu$
gradient	∇	∂_μ
trace	$\operatorname{tr}\Lambda$	$\Lambda^\mu{}_\mu$
tensor product	$T = x \otimes y$	$T^{\mu\nu} = x^\mu y^\nu$
$\vdots$	$\vdots$	$\vdots$

Occassionally, we will use Roman letters as indices, as in x^i. It is understood that Roman letters take values in $1, 2, 3$, whereas Greek ones take values in $0, 1, 2, 3$.

3.2 Relativistic wave equations

As a first step towards the construction of a full relativistic quatnum theory, we aim to guess a Poincaré-invariant substitute for the Schrödinger equation.

Let's recall the non-relativistic description of a single particle with mass m and no external potential (which would break translation symmetry). The solutions of the Schrödinger equation

$$\Big(i\partial_t - \frac{1}{2m}\sum_{i=1}^{3}\partial_{x_i}^2\Big)\psi(t,\vec{x}) = 0$$

are functions $\psi : \mathbb{R}^4 \to \mathbb{C}$ in the case of no spin, or $\psi : \mathbb{R}^4 \to \mathbb{C}^2$ for spin-$1/2$.

We aim to guess a relativistic generalization under the following assumptions (c.f. Appendix B), which should be plausible by anaology with the non-relativistic case:

- Quantum states and their time evolutions are described by (possibly vector-valued) functions $\psi(t, \vec{x})$ on space-time, which satisfy a linear differential equation

$$D\psi(t,\vec{x}) = 0, \tag{3.5}$$

  where D is some polynomial in the ∂_μ.

- The space of solutions of (3.5) is invariant under Poincaré transformations.

- Space-time translations $\tilde{x}^\mu = x^\mu + a^\mu$ act by shifting the wave functions:

$$\tilde{\psi}(\tilde{x}^\mu) = \psi(x^\mu - a^\mu). \tag{3.6}$$

- To interpret the solutions, we identify $i\partial_t$ with the energy operator, and $-i\,\partial_j$ with the operator measureing momentum in x_j-direction. This is sometimes called the *correspondence principle*.

- Based on the correspondence principle, and by analogy with the relativistic energy-momentum relation

$$E = \sqrt{m^2 + \|\vec{p}\|^2} \qquad \Rightarrow \qquad E^2 - \|\vec{p}\|^2 = m^2,$$

we will associate solutions ψ which satisfy the eigenvalue equation

$$\left(-\partial_t^2 + \partial_x^2 + \partial_y^2 + \partial_z^2\right)\psi = m^2\psi \tag{3.7}$$

with particles of (rest) mass m.

Most of the assumptions can be justified by analyzing the action of symmetry operations.

We won't describe the details here (but see Appendix **??** for more background). The relevant keywords to check for in the literature [**?**, **?**] are these: Using *Wigner's classification* or *Mackey's Machine*, one can argue that all physically relevant unitary representations of the Poincaré group are realized as actions on fields. Indeed, the translations form an Abelian subgroup of the Poincaré group. Thus, one can use eigenvectors of the translations as a basis of the representation space. Call this the *momentum eigenbasis*. After a Fourier transform, one obtains fields define on space-time. The Fourier transform of multiplication operators are shifts. This explains (3.6). The generators of shifts are differential operators. One can argue that generators of shifts transform in the way that is expected for energy-momentum observables, and thus arives at the corespondence principle. Finally, the formal Minkowski inner product of the energy-momentum translation generators with themselves are what is called a *Casimir operator* – an operator that is a multiple of the identity in every irreducible representation. Hence one can associate a scalar mass with any representation.

3.3 Klein-Gordon equation

Based on the correspondence principle and the energy-momentum relation, we posited that (3.7) characterizes solutions for particles of mass m. Our first attempt at guessing a relativistic wave equation is to just take D to be (3.7):

$$\left(\partial_\mu\partial^\mu - m^2\right)\psi = 0,$$

where

$$\partial_\mu\partial^\mu = \partial_t^2 - \partial_x^2 - \partial_y^2 - \partial_z^2 = \Box$$

is sometiemes called the *d'Alembertian*. As a contraction of a co- and a contravariant quantity, the d'Alembertian is *invariant* under Lorentz transformations (and hence under Poincaré transformations, as translations do not change differential operators).

The space of solutions is spanned by plane waves

$$\psi_{\vec{p}}^{\pm}(x^\mu) = e^{-ip_\mu x^\mu} \qquad \text{with} \qquad p_\mu = (\pm\omega_p, \vec{p}), \quad \omega_p = \sqrt{m^2 + |\vec{p}\|^2}, \tag{3.8}$$

indexed by momenta $\vec{p} \in \mathbb{R}^3$.

There are two problems with the KG-equation:

- The solutions ψ_p in (3.8) can have both positive and negative energy

$$i\partial_t \psi^{\pm}_{\vec{p}} = \pm\omega_p \, \psi^{\pm}_{\vec{p}}$$

  of arbitrary magnitude. The means particles could emit an unbounded amount of energy by transitioning into negative energy states. This, to put it mildly, is not observed.

- The KG equation does not have a natural positive local conserved quantity that could be interpreted as a probability.

> As a consequence of the energy operator being $E = i\partial_t$, *negative* energies are associated with *positive frequencies*!

TBD: Type up charge conservation.

It turns out that one can make sense of the KG equation by re-interpreting it as a kind of classical wave equation that needs to be quantized in the same way as we quantized the EM field.

To this end, write the field as a superposition

$$\begin{aligned}\phi(t,\vec{x}) &= \frac{1}{(2\pi)^{3/2}} \int \left(\phi^+(\vec{p})\psi^+_{\vec{p}}(t,\vec{x}) + \phi^-(\vec{p})\psi^-_{-\vec{p}}(t,\vec{x})\right) \frac{\mathrm{d}^3\vec{p}}{\sqrt{2\omega_p}} \\ &= \frac{1}{(2\pi)^{3/2}} \int \left(\phi^+(\vec{p})e^{-i\omega_p t + i\vec{p}\vec{x}} + \phi^-(\vec{p})e^{i\omega_p t - i\vec{p}\vec{x}}\right) \frac{\mathrm{d}^3\vec{p}}{\sqrt{2\omega_p}}\end{aligned}$$

of positive and negative energy solutions with coeffients $\phi^{\pm}(\vec{p}) \in \mathbb{C}$. We want to apply the free-field quantization scheme of Sec. 2.2. The difference compared to the EM case is that the field is complex, i.e. the expansion coefficients ϕ^+, ϕ^- are independent. We have to decide how to handle this independence, ideally in such a way that those pesty negative energies go away.

A choice that solves both issues is to associate one particle type with each of the independent components ϕ^+, ϕ^-. If we do it in such a way that negative frequencies are associated with annihilation operators, then the Hamiltonian will be positive. Indeed, set

$$\hat{\phi}(t,\vec{x}) = \frac{1}{(2\pi)^{3/2}} \int \left(a_{\vec{p}} e^{-i\omega_p t + i\vec{p}\vec{x}} + b^\dagger_{\vec{p}} e^{i\omega_p t - i\vec{p}\vec{x}}\right) \frac{\mathrm{d}^3\vec{p}}{\sqrt{2\omega_p}}, \tag{3.9}$$

where the $a_{\vec{k}}, b_{\vec{k}}$ are mutually commuting Bosonic annihilation operators. It is then trivial to check that (3.9) is the Heisenberg-picture time evolution for $\hat{\phi}(\vec{x}) = \hat{\phi}(t = 0, \vec{x})$ under

$$\hat{H} = \sum_{\vec{p}} \omega_p \left(a^\dagger_{\vec{p}} a_{\vec{p}} + b^\dagger_{\vec{p}} b_{\vec{p}}\right)$$

which obviously has non-negative eigenvalues.

TBD: type up charge conservation. More about interpretation.

3.4 Dirac equation

The Schrödinger equation

$$i\partial_t \psi = -\frac{1}{2m}\nabla^2\psi$$

mixes first order derivatibes in time with second order derivatives in space. The Klein-Gordon equation lifted the discrepancy by going second order in all coordinates. Here, we will seek to guess a Lorentz-invariant wave equation that is *first order* w.r.t. all coordinates:

$$\big(-i\gamma^\mu\partial_\mu + m\big)\psi = 0, \tag{3.10}$$

where the γ^μ have to be chosen so that the solutions "make physical sense".

3.4.1 Relativistic dispersion relation

Our first goal is to find the conditions on γ^μ so that the solutions of (3.10) fulfill the energy-momentum relation in the form of Eq. (3.7). It will turn out that *this is impossible* if ψ is taken to be a complex-valued function of space-time (as in the Klein-Gordon case). Dirac managed to circumvent this problem by going to *vector-valued* wave functions $\psi_i(x^\mu)$, $i = 1 \dots m$. The "coefficients" γ^μ then become $m \times m$ matrices.

The problem is easier to discuss in terms of the matrices

$$\beta := (\gamma^0)^{-1}, \qquad \alpha^i := (\gamma^0)^{-1}\gamma^i.$$

Then Eq. (3.10) becomes

$$i\gamma^0\partial_t\,\psi = -i\sum_{i=1}^{3}\gamma^i\partial_i\psi + m\psi \qquad \Leftrightarrow \qquad i\partial_t\,\psi = \underbrace{\Big(-i\sum_{i=1}^{3}\alpha^i\partial_i + m\beta\Big)}_{=:H}\psi. \tag{3.11}$$

Using (3.11) to eliminate ∂_t^2 in the energy-momentum relation (3.7), we get the condition

$$\begin{aligned}
&\Big(-i\sum_{i=1}^{3}\alpha^i\partial_i + m\beta\Big)^2 \\
&= -\sum_{i=1}^{3}(\alpha^i)^2\partial_i^2 + m^2\beta^2 - i\sum_{i\neq j=1}^{3}\big(\alpha^i\alpha^j + \alpha^j\alpha^i\big)\partial_i\partial_j - mi\sum_{i=1}^{3}\big(\alpha^i\beta + \beta\alpha^i\big)\partial_i \\
&\overset{!}{=} -\sum_{i=1}^{3}\partial_i^2 + m^2,
\end{aligned}$$

which is equivalent to

$$\{\alpha^i, \alpha^j\} = 2\delta_{ij}\,\mathbb{1}, \qquad \{\alpha^i, \beta\} = 0, \qquad \beta^2 = \mathbb{1}. \tag{3.12}$$

In terms of γ^μ, this is equivalent to

$$\{\gamma^\mu, \gamma^\nu\} = 2g^{\mu\nu}\,\mathbb{1}, \qquad (\gamma^\mu)^\dagger = (\gamma^\mu)^{-1} = g_{\mu\nu}\gamma^\nu. \tag{3.13}$$

In mathematical terms, the relations (3.13) say that the gamma matrices are generators of the *Clifford algebra* associated with the Minkowski metric. The rich theory of Clifford algebras places many of the constructions in this lecture in a much more general context. For example, such diverse topics as Bogoliubov transformations and the spinor representations of the Lorentz group arise there in a uniform way. We will not go into these more mathematical topics here, though.

Clearly, there is no solution to (3.13) if the γ^μ's are scalars. Are there any solutions at all? Well, anti-commuting matrices that square to $\mathbb{1}$ – where have we heard this before? Right – our old friends the Pauli matrices

$$\mathbb{1} = \sigma_0 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \qquad X = \sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix},$$
$$Y = \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \qquad Z = \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

have this property. One minor problem: there's only three non-trivial Pauli matrices, while we need *four* γ matrices. To get around this, we consider tensor products of Paulis. Indeed, it is easy to verify that one solution to (3.13) is

$$\begin{aligned} \gamma^0 &= Z \otimes \mathbb{1}, \\ \gamma^1 &= i\, Y \otimes X, \\ \gamma^2 &= i\, Y \otimes Y, \\ \gamma^3 &= i\, Y \otimes Z. \end{aligned}$$

With respect to the tensor product basis $|++\rangle, |+-\rangle, |-+\rangle, |--\rangle$, we have

$$\gamma^0 = \begin{pmatrix} \mathbb{1} & 0 \\ 0 & -\mathbb{1} \end{pmatrix}, \qquad \gamma^i = \begin{pmatrix} 0 & \sigma_i \\ -\sigma_i & 0 \end{pmatrix},$$

We have found the *Dirac representation* of the γ-matrices!

Many other representations exist. They are all requivalent to each other in a precise sense – but different representations are used for different applications. In addition to the one found by Dirac, we will also employ the *Weyl* or *chiral* representation, which starts from

$$\begin{aligned} \gamma^0 &= X \otimes \mathbb{1}, \\ \gamma^1 &= i\, Y \otimes X, \\ \gamma^2 &= i\, Y \otimes Y, \\ \gamma^3 &= i\, Y \otimes Z, \end{aligned}$$

respectively

$$\gamma^0 = \begin{pmatrix} 0 & \mathbb{1} \\ \mathbb{1} & 0 \end{pmatrix}, \qquad \gamma^i = \begin{pmatrix} 0 & \sigma_i \\ -\sigma_i & 0 \end{pmatrix}, \qquad \gamma^5 = \begin{pmatrix} -\mathbb{1} & 0 \\ 0 & \mathbb{1} \end{pmatrix},$$

in the above basis.

We have thus found the *Dirac equation*

$$\big(-i\gamma^\mu \partial_\mu + m\big)\psi = 0$$

in terms of the vector-valued wave function

$$\psi(x^\mu) = \begin{pmatrix} \psi_1(x^\mu) \\ \psi_2(x^\mu) \\ \psi_3(x^\mu) \\ \psi_4(x^\mu) \end{pmatrix},$$

which is called the *(Dirac) spinor*. The term *spinor* is a *portmanteau* (i.e. a contraction of two words) shortening "spin vector".

At this point, we have no idea how to interpret the four components of spinor. As a first step, we'll work out how spinors transform under Lorentz transformations.

3.4.2 The action of the Lorentz group on spinors

Recall the general transformation law of vector fields, Eq. (3.4). Thus, given spinor field ψ and a Lorentz transformation Λ, the spinor field $\tilde{\psi}$ displaced by Λ is of the form

$$\tilde{\psi}(\cdot) = S_\Lambda \psi(\Lambda^{-1}\cdot)$$

for some 4×4-matrix S_Λ to be determined.

The only guidance we have for finding these matrices is that $\tilde{\psi}$ must solve the Dirac equation if and only if ψ does. We first try to find an S_Λ that does not depend on the space-time point x^μ (so that it commutes with differential operators). Fortunately, such a solution does exist, so we never have to consider the more general case.

Indeed, under Λ, the Dirac equation transforms as

$$\begin{aligned} & i\gamma^\mu \tilde{\partial}_\mu \tilde{\psi} = m\tilde{\psi} \\ \Leftrightarrow \quad & i\gamma^\mu \tilde{\partial}_\mu S_\Lambda \psi = m S_\Lambda \psi \\ \Leftrightarrow \quad & i\big(S_\Lambda^{-1}\gamma^\mu S_\Lambda\big)\tilde{\partial}_\mu \psi = m\psi. \end{aligned}$$

We want left hand side to be equal $i\gamma^\mu \partial_\mu \psi$. Since the derivatives transform covariantly, this is equivalent to demanding that the expression in paranthesis transforms contravariantly:

$$S_\Lambda^{-1}\gamma^\mu S_\Lambda = \Lambda^\mu{}_\alpha \gamma^\alpha. \tag{3.14}$$

It is not obvious that matrices S_Λ with the property (3.14) exist. To clarify this, we have to dive a bit deeper into the structure of the Lorentz group.

The connected components of the Lorentz group

Recall that a 4×4 matrix Λ is an element of the Lorentz group $O(1,3)$ if and only

$$\Lambda^T g \Lambda = g. \tag{3.15}$$

We'll use (3.15) to identify four components of the Lorentz group. First, taking determinants,

$$\det\Lambda \, \det g \, \det\Lambda = \det g \qquad \Rightarrow \qquad \det\Lambda = \pm 1.$$

Transformations Λ with determinant $+1$ are called *proper*. Next, consider the 0-0 component of the transformation law:

$$1 = \left(\Lambda^T g \Lambda\right)_{00} = \Lambda^\mu{}_0 g_{\mu\nu} \Lambda^\nu{}_0 = (\Lambda^0{}_0)^2 - \sum_{i=1}^{3} (\Lambda^i{}_0)^2.$$

Because the second summand is non-positive, this condition implies $\Lambda_{00} \neq 0$, and we conclude the the sign $(\Lambda^0{}_0) \in \pm 1$ is well-defined. Transformations Λ with positive sign are called *orthochronus*. We have thus identified four components of the Lorentz group that cannot be continoulsy connected. It turns out that this is finest such decompostion, i.e. there are exactly four *connected components* (Fig. **??**). Only one of them contains the identity and is thus a group in its own right: the proper orthochronus (or *restricted*) Lorentz group $\mathrm{SO}^+(1,3)$.

We will construct the spinor representation of $\mathrm{SO}^+(1,3)$ in two different ways: explicitly in terms of generators in Section 3.4.2, and then indirectly in Sec. 3.4.2. It is sufficient to understand either of the two approaches.

Explicit form of the spinor representation

TBD — this is a placeholder — TBD

Generators of the Lorentz group:

$$\omega^{\mu\nu} = \begin{pmatrix} 0 & k_1 & k_2 & k_3 \\ k_1 & 0 & j_3 & j_1 \\ k_2 & -j_3 & 0 & j_2 \\ k_3 & -j_1 & -j_2 & 0 \end{pmatrix}. \tag{3.16}$$

The commutation relation can be worked out explicitly For the record:

$$\begin{aligned} [J_1, J_2] &= iJ_3 \qquad \text{(and cyclic permutations of indices)}, \\ [K_1, J_2] &= iK_3 \qquad \text{(and cyclic permutations of indices)}, \\ [K_1, K_2] &= -iJ_3 \qquad \text{(and cyclic permutations of indices)}. \end{aligned}$$

These are represented by

$$\omega^{\mu\nu} \mapsto S^{\mu\nu} = \frac{i}{4}[\gamma^\mu, \gamma^\nu].$$

In Weyl representation, this gives for the boosts

$$K_i = S^{0i} = -\frac{i}{2} \begin{pmatrix} \sigma^i & 0 \\ 0 & -\sigma^i \end{pmatrix}$$

and for the rotations

$$J_k = S^{ij} = \frac{1}{2} \begin{pmatrix} \sigma^k & 0 \\ 0 & \sigma^k \end{pmatrix} \qquad (ijk) \text{ cyclic}.$$

Clearly, the representation decomposes. The upper one turns out to coincide with the left-handed spinor representation, while the lower one is the right-handed spinor representation.

Hence

$$\exp\big(i(k^i K_i + j^k J_k)\big) = \exp\big(-\frac{1}{2}k^i\sigma^i + \frac{i}{2}j^k\sigma^k\big) \oplus \exp\big(+\frac{1}{2}k^i\sigma^i + \frac{i}{2}j^k\sigma^k\big)$$
$$= A^{(L)} \oplus A^{(R)}$$

and

$$(A^{(L)})^{-\dagger} = \exp\big(+\frac{1}{2}k^i\sigma^i + \frac{i}{2}j^k\sigma^k\big) = A^{(R)}.$$

From (3.16), the contragredient corresponds to

$$k_i \to -k_i, \qquad j_i \to j_i$$

so $A^{(L)}(\Lambda) = A^{(R)}(\Lambda^{-T})$.

Minkowski space as Hermitian 2×2 matrices

Let's introduce a cool trick for implicitly constructing the spinor representation. The four Pauli matrices form a basis of the space of Hermitian 2×2 matrices. We can thus map covariant 4-vectors onto matrices via:

$$x_\mu \mapsto x_\mu\sigma^\mu = \begin{pmatrix} x_0 + x_3 & x_1 - ix_2 \\ x_1 + ix_2 & x_0 - x_3 \end{pmatrix}. \tag{3.17}$$

(This is an extension of the *Bloch sphere* representation of 2×2 density matrices that you will recall from elementary QM). The cool coincidence which makes this representation important is that the determinant turns out to be the Minkowski norm:

$$\det x_\mu\sigma^\mu = \det \begin{pmatrix} x_0 + x_3 & x_1 - ix_2 \\ x_1 + ix_2 & x_0 - x_3 \end{pmatrix} = (x_0)^2 - (x_3)^2 - (x_1)^2 - (x_2)^2 = x_\mu x^\mu.$$

Now fix some complex 2×2 matrix $A \in SL(2, \mathbb{C})$ of determinant one and consider the map

$$x \mapsto A\, x_\mu\sigma^\mu A^\dagger. \tag{3.18}$$

Because the result is again Hermitian, and because the Paulis form a basis,

$$A\, x_\mu\sigma^\mu A^\dagger = y_\mu\sigma^\mu$$

for some y_μ. Because (3.18) is linear, there is some 4×4 matrix Λ s.t. $y = \Lambda^{-t}x$ (the action on co-vectors), i.e.

$$A\, x_\mu\sigma^\mu A^\dagger = \Lambda_\mu{}^\nu x_\nu.$$

Now comes the central step. Because

$$y_\mu y^\mu = \det A\, x_\mu\sigma^\mu A^\dagger = \det x_\mu\sigma^\mu = x_\mu x^\mu,$$

the matrix Λ is actually an element of the Lorentz group! Because the set of determinant-one complex matrices is connected, Λ has to be proper and orthochronus. We thus obtain an important map $\mathrm{SL}(2, \mathbb{C}) \to \mathrm{SO}^+(1, 3)$.

The proper orthochronus Lorentz group has six real parameters (3 for rotations and 3 for boosts). The same holds for $\mathrm{SL}(2,\mathbb{C})$ (a complex 4×4 matrix has eight, but the $\det = 1$ condition removes one complex = two real parameters). It is thus plausible to assume – and indeed true – that the map is onto, i.e. that every Lorentz transformation $\Lambda \in SO^+(1,3)$ can be realized by a complex matrix A. In fact, as A and $-A$ clearly have the same determinant and induce the same Λ, the map $\mathrm{SL}(2,\mathbb{C}) \to \mathrm{SO}^+(1,3)$ is two-to-one. This is connected with the deep and exciting fact that the wave function of particles with half-integer spin picks up a sign of -1 after a 360° rotation. This ambiguity will not be important for our purposes here, as (3.18) is *quadratic* in the A's, so that factors of -1 cancel. Thus, we will get away with writing

$$\Lambda \mapsto A_\Lambda$$

for one of the two A's associated with Λ, without specifying which one is meant. This is called the *left-handed spinor representation*, for reasons that we'll learn about soon.

The name suggests that there's a *right-handed spinor* represenation. It follows from a general construction: Recall that 4-vectors transform under Λ, whereas co-vectors transform under Λ^{-T}. In general, because

$$(AB)^{-\dagger} = A^{-\dagger}B^{-\dagger},$$

taking the transpose-dagger of any matrix group gives again a group. This is called the *contragredient* representation. In quantum mechanics, we are usually concerned with *unitary* groups, for which no new group arises this way (because $U^{-\dagger} = U$). But our A's here are not necessarily untiary, so the contragredient

$$\Lambda \mapsto A_\Lambda^{-\dagger}$$

is a different representation of the Lorentz group – the *right-handed spinor representation*. It is plausible and indeed true (see below) that

$$A_\Lambda^{-\dagger} = A_{\Lambda^{-T}},$$

i.e. the contragredient of Λ is represented by the contragredient of A_Λ.

Transformation law for spinors: The relevance of the above construction for spinors becomes clear if we write out the matrix representation of a linear combination of γ-matrices in the Weyl representation. For a covariant vector x_μ:

$$x_\mu\gamma^\mu = \begin{pmatrix} 0 & x_\mu\sigma^\mu \\ (Px)_\mu\sigma^\mu & 0 \end{pmatrix},$$

where

$$P = \begin{pmatrix} 1 & 0 \\ 0 & -\mathbb{1} \end{pmatrix}$$

is the parity operation that inverts spatial coordinates. If we define the *parity-inverted Pauli matrices* as

$$\bar\sigma^0 = \sigma^0, \qquad \bar\sigma^i = -\sigma^i$$

then

$$x_\mu \gamma^\mu = \begin{pmatrix} 0 & x_\mu \sigma^\mu \\ x_\mu \bar{\sigma}^\mu & 0 \end{pmatrix},$$

Set

$$S_\Lambda = \begin{pmatrix} A_\Lambda & 0 \\ 0 & A_\Lambda^{-\dagger} \end{pmatrix}.$$

Using (**??**), $P = g = g^{-1}, P^2 = \mathbb{1}$, we get

$$\Lambda^{-1} P = P P \Lambda^{-1} P = P \Lambda^T$$

so that

$$\begin{aligned} S_\Lambda^{-1} x_\mu \gamma^\mu S_\Lambda &= \begin{pmatrix} A_\Lambda^{-1} & 0 \\ 0 & A_\Lambda^\dagger \end{pmatrix} \begin{pmatrix} 0 & x_\mu \sigma^\mu \\ x_\mu \bar{\sigma}^\mu & 0 \end{pmatrix} \begin{pmatrix} A_\Lambda & 0 \\ 0 & A_\Lambda^{-\dagger} \end{pmatrix} \\ &= \begin{pmatrix} 0 & A_{\Lambda^{-1}} x_\mu \sigma^\mu A_{\Lambda^{-1}}^\dagger \\ A_\Lambda^\dagger x_\mu \bar{\sigma}^\mu A_\Lambda & 0 \end{pmatrix} \\ &= \begin{pmatrix} 0 & (\Lambda^T x)_\mu \sigma^\mu \\ (\Lambda^{-1} P x)_\mu \sigma^\mu & 0 \end{pmatrix} \\ &= \begin{pmatrix} 0 & (\Lambda^T x)_\mu \sigma^\mu \\ (P \Lambda^T x)_\mu \sigma^\mu & 0 \end{pmatrix} \\ &= \begin{pmatrix} 0 & (\Lambda^T x)_\mu \sigma^\mu \\ (\Lambda^T x)_\mu \bar{\sigma}^\mu & 0 \end{pmatrix}. \end{aligned}$$

But

$$(\Lambda^T x)_\mu \sigma^\mu = x_\nu \Lambda^\nu{}_\mu \sigma^\mu$$

and likewise for the parity-inverted version. Comparision with Eq. (3.14) shows that spinors in Weyl representation transform under S_Λ as defined here!

Note that S_Λ is *not* unitary. It is still true, though, that inverse and adjoint are closely related:

$$S_\Lambda^{-1} = \begin{pmatrix} A_\Lambda^{-1} & 0 \\ 0 & A_\Lambda^\dagger \end{pmatrix} = \begin{pmatrix} A_\Lambda^{-1} & 0 \\ 0 & A_\Lambda^\dagger \end{pmatrix}^\dagger \begin{pmatrix} 0 & \mathbb{1} \\ \mathbb{1} & 0 \end{pmatrix} = S_\Lambda^\dagger \gamma^0.$$

Solutions of the Dirac equation: It becomes apparent that the restricted Lorentz group leaves the first two and the last two coordinates invariant. They are called *left- and right-handed Weyl spinors* and it makes sense to set

$$\psi = \begin{pmatrix} \psi_L \\ \psi_R \end{pmatrix}$$

With this notation, the Dirac equation becomes

$$(i\gamma^\mu \partial_\mu - m)\psi = \begin{pmatrix} -m & i(\partial_0 + \vec{\sigma} \cdot \vec{\nabla}) \\ i(\partial_0 - \vec{\sigma} \cdot \vec{\nabla}) & -m \end{pmatrix} \begin{pmatrix} \psi_L \\ \psi_R \end{pmatrix} = 0.$$

Consider first the massless case (thought to describe neutrinos, until their mass was discovered). Then the Dirac equation decouples into the *Weyl equations*

$$i(\partial_t - \vec{\sigma}\cdot\vec{\nabla})\psi_L = 0, \qquad i(\partial_t\psi_R + \vec{\sigma}\cdot\vec{\nabla})\psi_R = 0.$$

Define the *helicity operator*

$$h = \vec{\sigma}\cdot\frac{\vec{P}}{\|\vec{P}\|}$$

to be the projection of spin onto direction of travel. For eigenfunctions of a massless particle, $\|\vec{P}\| = E$, so that

$$Eh = \vec{\sigma}\cdot\vec{P} = -i\vec{\sigma}\cdot\vec{\nabla}.$$

Thus the Weyl equations imply for eigenfunctions

$$\begin{aligned} E + Eh = 0 \quad &\Rightarrow \quad h = -1 \qquad \text{(left-handed)} \\ E - Eh = 0 \quad &\Rightarrow \quad h = +1 \qquad \text{(right-handed)}. \end{aligned}$$

To $\gamma^0, \ldots, \gamma^3$ one usually adds another gamma matrix:

$$\gamma^5 := i\gamma^0\gamma^1\gamma^2\gamma^3 = X \otimes \mathbb{1} = \begin{pmatrix} -\mathbb{1} & 0 \\ 0 & \mathbb{1} \end{pmatrix}.$$

(The fact that the 4th matrix is called γ^5 is neither a bad joke nor a typo, but a historic artifact stemming from a convention that labelled space-time vectors with indices 1 through 4...). Then the helicity operator h is just γ^5 and the projections onto the left- and right-handed eigenspaces are given by

$$P_{L/R} = \frac{1}{2}(\mathbb{1} \mp \gamma^5).$$

The utility of this formula is that it holds in any representation for the gamma matrices.

In general, separating variables, we may assume that solutions are of the form

$$\psi(x^\mu) = \begin{pmatrix} \psi_L(p) \\ \psi_R(p) \end{pmatrix} e^{-ip_\mu x^\mu}.$$

Assume for now that $p_0 > 0$. We can use a Loretnz transform to "switch into the frame of reference where the particle is at rest", i.e. up to a Lorentz transformation, we may assume that $p = (m, 0)$. Then the spatial derivatives vanish, so the equation for the $\psi_{L/R}$ becomes

$$m\begin{pmatrix} -\mathbb{1} & \mathbb{1} \\ \mathbb{1} & -\mathbb{1} \end{pmatrix}\begin{pmatrix} \psi_L(p) \\ \psi_R(p) \end{pmatrix} = 0 \quad \Leftrightarrow \quad \psi_L(p) = \psi_R(p). \tag{3.19}$$

Thus, for massive particles, the four components of the spinor are actually redundant! Only two of them can be chosen freely. Of course, also in a reference frame where the particle is not at rest, only two parameters are free. However, the relation is not in general as simple as (3.19).

Using the explicit form of the spinor representation (Sec. 3.4.2), one can work out a relatively simple formula for the spinor representation of a Lorentz group element that maps the rest-frame solution $\alpha = (m, 0, 0, 0)$ to an arbitrary one $\beta = (E, \vec{p})$.
For the boost, compute:

$$e^{\eta K^3} = \begin{pmatrix} \cosh(\eta) & \sinh(\eta) \\ \sinh(\eta) & \cosh(\eta) \end{pmatrix} \qquad (x \text{ and } y \text{ coordinates not shown}).$$

so that

$$e^{\eta K^3} \begin{pmatrix} m \\ 0 \end{pmatrix} = \begin{pmatrix} \cosh(\eta) & \sinh(\eta) \\ \sinh(\eta) & \cosh(\eta) \end{pmatrix} \begin{pmatrix} m \\ 0 \end{pmatrix} = \begin{pmatrix} m\cosh(\eta) \\ m\sinh(\eta) \end{pmatrix} = \begin{pmatrix} E \\ p_z \end{pmatrix}$$

and hence

$$E \pm p_z = m(\cosh\eta \pm \sinh\eta) = m\, e^{\pm\eta}.$$

Find a $\tilde{\Lambda}$ that maps $\alpha = (m, 0)$ to $\beta = (\omega_p, \vec{p})$. With $q_i = p_i/\|\vec{p}\|^2$:

$$\tilde{\Lambda} = \begin{pmatrix} \cosh\eta & \sinh\eta \vec{q}^T \\ \sinh\eta\vec{q} & \cosh\eta\vec{q}\vec{q}^T \end{pmatrix}, \qquad \tilde{\Lambda}^{-T} = \begin{pmatrix} \cosh\eta & -\sinh\eta \vec{q}^T \\ -\sinh\eta\vec{q} & \cosh\eta\vec{q}\vec{q}^T \end{pmatrix}.$$

Hence

$$\hat{E} = -(\tilde{\Lambda}^{-T}\alpha)_0 = -m\cosh\eta, \qquad \hat{\vec{P}} = -(\tilde{\Lambda}^{-T}\alpha) = \sinh\eta\,\vec{q}.$$

With $p = (E, 0, 0, p_z)$,

$$e^{-\frac{1}{2}\eta\sigma^3} = \begin{pmatrix} e^{-\eta/2} & 0 \\ 0 & e^{\eta/2} \end{pmatrix} = \frac{1}{\sqrt{m}} \begin{pmatrix} \sqrt{E-p_z} & 0 \\ 0 & \sqrt{E+p_z} \end{pmatrix} = \sqrt{\frac{1}{m} p_\mu \sigma^\mu},$$

where the square root acts on the eigenvalues of the matrix. For the right-handed spinors:

$$e^{+\frac{1}{2}\eta\sigma^3} = \frac{1}{\sqrt{m}} \begin{pmatrix} \sqrt{E+p_z} & 0 \\ 0 & \sqrt{E-p_z} \end{pmatrix} = \sqrt{\frac{p}{m} \cdot \bar{\sigma}} = \sqrt{\frac{1}{m} p_\mu \bar{\sigma}^\mu},$$

The final formula is valid for a boost in any direction, not just along the z-axis.

Non-relativistic approximation

It is very fruitful to consider the Dirac equation in the non-relativistic limit, where energies are small compared to the rest mass.

Dirac equation with fields: We will treat that limit for a version of the Dirac equation which incorporates classical EM fields. Recall that in classical Hamiltonian mechnics, as well as in non-relativistic QM, one passes from a free particle to one that is subject to classical fields via the substitution (*minimal copuling*):

$$H = \frac{1}{2m}\vec{P}^2 \qquad \mapsto \qquad H = \frac{1}{2m}(\vec{P} - q\vec{A})^2 + q\phi.$$

In terms of the Schrödinger equation:

$$\big(i\partial_t - \frac{1}{2m}(-i\hat{\nabla})^2\big)\psi = 0 \qquad \mapsto \qquad \big(i\partial_t - q\phi - \frac{1}{2m}(-i\hat{\nabla} - q\vec{A})^2\big)\psi = 0$$

Which can be summarized in covariant notation as

$$p_\mu \mapsto p_\mu - qA_\mu \quad \text{i.e.} \quad i\partial_\mu \mapsto i\partial_\mu - qA_\mu.$$

The (contravariant) potential four-vector is $A^\mu = (\phi, \vec{A})$. Thus, $A_\mu = (\phi, -\vec{A})$. We will use the symbol $\vec{A}_i$, with a vector sign and a Roman subscript to denote the components of the three-vector $\vec{A}$ – which are thus *minus* the spatial components of the covariant A_μ.

Thus, we might guess (correctly, as it turns out) that

$$\big(-\gamma^\mu (i\partial_\mu - qA_\mu) + m\big)\psi = 0 \tag{3.20}$$

is the right form of the Dirac equation in the presence of fields.

Dirac equation in Dirac representation (I know...): It turns out that the non-relativistic limit is best treated in Dirac representation. Denote the components of the Dirac spinor as $\psi = (\psi_l, \psi_s)$, with $\psi_{l/s} \in \mathbb{C}^2$. The subscripts l and s stand for "large" and "small", for reasons that will become clear momentarily. With these conventions, Eq. (3.20) reads

$$(i\partial_t - q\phi)\begin{pmatrix}\psi_l \\ -\psi_s\end{pmatrix} = \sum_{j=1}^{3}\begin{pmatrix}0 & -\sigma^j(i\partial_j + q\vec{A}_j) \\ \sigma^j(i\partial_j + q\vec{A}_j) & 0\end{pmatrix}\begin{pmatrix}\psi_l \\ \psi_s\end{pmatrix} + m\begin{pmatrix}\psi_l \\ \psi_s\end{pmatrix}.$$

Setting

$$\vec{\sigma} = (\sigma^1, \sigma^2, \sigma^3), \qquad \vec{\Pi} = \vec{p} - q\vec{A},$$

so that

$$\sum_{j=1}^{3}\sigma^j(-i\partial_j - q\vec{A}_j) = \vec{\sigma}\vec{\Pi},$$

we arrive at the two coupled equations

$$i\partial_t\psi_l = \vec{\sigma}\vec{\Pi}\,\psi_s + (m + q\phi)\psi_l \tag{3.21}$$

$$i\partial_t\psi_s = \vec{\sigma}\vec{\Pi}\,\psi_l + (-m + q\phi)\psi_s. \tag{3.22}$$

Solutions in the non-relativisitic limit: As a linear partial differential equation (3.20) allows for a complete set of solutions in terms of plane waves

$$\psi(x^\mu) = \begin{pmatrix}\psi_l \\ \psi_s\end{pmatrix} e^{-ip_\mu x^\mu}.$$

With $E = p^0$, Eq. (3.22) evaluated on such a plane wave gives

$$\psi_s = \frac{1}{E + m - q\phi}\vec{\sigma}\vec{\Pi}\psi_l. \tag{3.23}$$

Now we assume that we are in the non-relativistic limit where all energies are small compared ot the rest mass:

$$E - m \ll m, \qquad |qA_\mu| \ll m, \qquad |\partial_i\psi| \ll m|\psi|, \qquad \ldots$$

Then

$$E + m - q \simeq 2m,$$

so that

$$|\psi_s| \simeq \frac{1}{2m}\left|\vec{\sigma}\vec{\Pi}\psi_l\right| \leq \frac{1}{2m}\Big(\sum_{j=1}^{3}|\partial_j\psi_l| + |qA_j\psi_l|\Big) \ll |\psi_l|.$$

Thus, in the non-relativistic regime, the "small spinor" ψ_s has a much smaller norm than the "large spinor" ψ_l and can therefore be neglected. In order to eliminate ψ_s from the equations of motion, plug (3.23) into (3.21) to get

$$(E-m)\psi_l = \frac{1}{2m}\big(\vec{\sigma}\vec{\Pi}\big)^2\psi_l + q\phi\,\psi_l,$$

the *Pauli equation*.

Let's rephrase this:

$$\big(\vec{\sigma}\vec{\Pi}\big)^2 = \sum_{jk}\sigma_j\sigma_k\,\Pi_j\Pi_k = \sum_j \Pi_j^2 + i\sum_{jkl}\epsilon_{jkl}\sigma_l\,\Pi_j\Pi_k.$$

Compute the second summand for the case $l=3$:

$$\begin{aligned} i\sum_{jk}\epsilon_{jk3}\sigma_3\,\Pi_j\Pi_k &= i\sigma_z\big(\Pi_1\Pi_2 - \Pi_2\Pi_1\big) \\ &= -q\sigma_z\big(\partial_x\vec{A}_y + \vec{A}_x\partial_y - \partial_y\vec{A}_x - \vec{A}_y\partial_x\big) \\ &= -q\sigma_z\big(\partial_x\vec{A}_y\big) + q\sigma_z\big(\partial_y\vec{A}_x\big) = -q\sigma_3(\vec{\nabla}\times\vec{A}\big)_3. \end{aligned}$$

> Recall that we are working with operators! So $\partial_x A_y$ is *not* the x-derivative of A_y, but the operator that will act on a function ψ first by multiplying with A_y and then differentiating the product. Thus
>
> $$\big(\partial_x\vec{A}_y - \vec{A}_y\partial_x\big)\psi = \partial_x\big(\vec{A}_y\psi\big) - \vec{A}_y\partial_x\psi = \big(\partial_x\vec{A}_y\big)\psi + \vec{A}_y\partial_x\psi - \vec{A}_y\partial_x\psi = \big(\partial_x\vec{A}_y\big)\psi.$$

A similar calculation for the two other components gives

$$\big(\vec{\sigma}\vec{\Pi}\big)^2 = \sum_j(-i\partial_j - q\vec{A}_j)^2 - q\vec{\sigma}\cdot\big(\vec{\nabla}\times\vec{A}\big) = \big(\hat{\vec{P}} - q\vec{A}\big)^2 - q\vec{\sigma}\cdot\vec{B}.$$

Let

$$\vec{S} = \frac{1}{2}\vec{\sigma}, \qquad \mu_B = \frac{q}{2m}, \qquad g = 2$$

be the vector whose i-th component is the operator corresponding to the i-th spin direction, the *Bohr magneton*, and, respectively the g-factor. Thus:

$$(E-m)\psi_l = \left(\frac{1}{2m}\big(\hat{\vec{P}} - q\vec{A}\big)^2 + q\phi - g\mu_B\vec{S}\cdot\vec{B}\right)\psi_l.$$

Why did we break up the coupling constant $q/(2m)$ into two factors μ_B times g? To explain that, assume the magnetic field is constant and of the form

$$\vec{B} = \begin{pmatrix}0\\0\\B\end{pmatrix}.$$

A potential giving rise to this is

$$\vec{A} = \frac{1}{2}\vec{B} \times \vec{X} = \frac{1}{2}\begin{pmatrix} -By \\ Bx \\ 0 \end{pmatrix}.$$

Then

$$\big(-i\vec{\nabla} - q\vec{A}\big)^2 = -\vec{\nabla}^2 + iq\big(\vec{\nabla}\cdot\vec{A} + \vec{A}\cdot\vec{\nabla}\big) + q^2\vec{A}^2$$

For the middle summand, realize that A_i commutes with ∂_i so that it can be written as

$$-2q\vec{A}\cdot(-i\vec{\nabla}) = -q\big(xP_y - yP_x\big)B = -q\vec{L}\cdot\vec{B},$$

with *orbital angular momentum operator* $\vec{L} = \vec{X} \times \vec{P}$. Thus the Hamiltonian is

$$\begin{aligned} &\frac{1}{2m}\hat{\vec{P}}^2 - \frac{q}{2m}\big(\vec{L} + 2\vec{S}\big)\cdot\vec{B} + q\phi + \frac{1}{2m}\|\vec{B}\times\vec{X}\|^2 \\ \simeq &\frac{1}{2m}\hat{\vec{P}}^2 - \frac{q}{2m}\big(\vec{L} + 2\vec{S}\big)\cdot\vec{B} + q\phi, \end{aligned}$$

where the approximation holds when the magnetic field can be neglected to second order. Thus, whereas $\vec{L} + \vec{S}$ is a conserved quantity, the dynamical coupling between spin and magnetic field is twice as strong as between orbital angular and magnetic field!

Appendix A

QM recap

In this chapter, we recall some facts that should be familiar from linear algebra and introductory quantum mechanics courses. The textbook *Quantum Mechanics* by L. Ballentine is a good source for this material.

A.1 Linear algebra of Hilbert spaces

A.1.1 Hilbert spaces

A *Hilbert space* $\mathcal{H}$ is a complex vector space with a *sesquilinear* inner product $\langle\cdot|\cdot\rangle$. Sesquilinearity means that for all vectors

$$\alpha, \beta, \gamma \in \mathcal{H}$$

and complex numbers $z \in \mathbb{C}$, we have

$$\langle\alpha|\beta+\gamma\rangle = \langle\alpha|\beta\rangle + \langle\alpha|\gamma\rangle, \tag{A.1}$$
$$\langle\alpha|z\beta\rangle = z\langle\alpha|\beta\rangle, \tag{A.2}$$

as well as

$$\langle\alpha|\beta\rangle = \overline{\langle\beta|\alpha\rangle}. \tag{A.3}$$

From this, it follows that

$$\langle\alpha+\beta|\gamma\rangle = \langle\alpha|\gamma\rangle + \langle\beta|\gamma\rangle, \tag{A.4}$$
$$\langle z\alpha|\beta\rangle = \bar{z}\langle\alpha|\beta\rangle, \tag{A.5}$$

i.e. the inner product is anti-linear w.r.t. the first entry and linear w.r.t. the second one.

> Beware that mathematicians usually employ the opposite convention, where the sesquilinear inner product is linear in the first entry!

The *norm* of a vector $\alpha \in \mathcal{H}$ is given by

$$\|\alpha\| := \sqrt{\langle\alpha|\alpha\rangle}.$$

Recall that inner products are required to be *definite*, i.e. to fulfill

$$\|\alpha\| > 0 \quad \forall\alpha \neq 0.$$

There are two examples of Hilbert spaces you should be acquainted with: *column vectors* and *square-integrable functions*. Let's look at both in turn.

The vector space $\mathbb{C}^d$ is formed by d-dimensional complex column vectors of the form

$$\alpha = \begin{pmatrix} \alpha_1 \\ \vdots \\ \alpha_d \end{pmatrix}$$

with sesquilinear inner product

$$\langle \alpha | \beta \rangle = \sum_{i=1}^{d} \bar{\alpha}_i \beta_i. \tag{A.6}$$

It appers e.g. in the description of spin degrees of freedom.

More interesting is the Hilbert space $L^2(\mathbb{R}^n)$ of square-integrable complex functions on $\mathbb{R}^n$. Given two functions $\alpha, \beta : \mathbb{R}^n \to \mathbb{C}$, we can define a "continuous analogue" of Eq. (A.6):

$$\langle \alpha | \beta \rangle = \int \bar{\alpha}(x) \beta(x) \, \mathrm{d}^n x. \tag{A.7}$$

For the non-pedantic physicist, the space of all wave functions, together with (A.7) defines a Hilbert space. It is associated with a point particle with n degrees of freedom.

> There are three technical problems that one has to address to define the Hilbert space of functions with mathematical rigor.
>
> The first problem is the integral is not actually defined for all functions. Set, for example
>
> $$\psi(x) = \begin{cases} \sin(1/x) & x \neq 0, \\ 0 & x = 0. \end{cases}$$
>
> Then
>
> $$\int |\alpha(x)|^2 \, \mathrm{d}^n x$$
>
> does not exist (in either the Riemann or the Lesbeque sense). The second problem is that the integral may be defined, but infinite – take e.g. $\alpha(x) = 1$ and compute $\langle \alpha | \alpha \rangle$. To get rid of both problems, we define a function α to be *square-integrable* if
>
> $$\|\alpha\|^2 = \langle \alpha | \alpha \rangle = \int |\alpha(x)|^2 \, \mathrm{d}^n x$$
>
> exists and is finite. If α, β are square-integrable, then the product $\bar{\alpha}\beta$ is integrable, and the *Cauchy-Schwarz inequality* says that
>
> $$|\langle \alpha | \beta \rangle|^2 \leq \|\alpha\|^2 \, \|\beta\|^2 < \infty,$$
>
> so that, by restricting to square-integrable functions, we have rid outselves of undefined and infinite integrals!
>
> The third problem is that the norm is no longer definite. Indeed, define a function
>
> $$\alpha(x) = \begin{cases} 1 & x = 0 \\ 0 & x \neq 0 \end{cases}.$$

Then $\alpha \neq 0$, but $\|\alpha\|^2 = 0$. Circumventing this problem requires some mathematical gymnastics: We say that two functions are *equivalent* if they differ only on a set of measure zero. This means e.g. that the function α is equivalent to the 0-function, as the two differ only at one point. If we define the Hilbert space $L^2(\mathbb{R}^n)$ to be the *complex vector space of equivalence classes* of square-integrable functions, then one can show that (A.7) becomes a *definite* inner product. Problem solved.

A.1.2 Dirac notation

Physicists often use notational aids to delinate vector-valued quantities from scalars. In quantum mechanics, the suggestive *Dirac* notation (or "bra-ket" notation) is usually employed. Here, a vector $\alpha \in \mathcal{H}$ is written as $|\alpha\rangle$. This is called a *ket*, for reasons that will be obvious momentarily.

Every vector $\psi \in \mathcal{H}$ defines a linear function

$$\mathcal{H} \to \mathbb{C}, \qquad \phi \mapsto \langle\psi|\phi\rangle,$$

the "projection onto ψ". In quantum, we denote this function as $\langle\psi|$ and call it a *bra*. Then we can write

$$\langle\psi|(|\phi\rangle) = \langle\psi|\phi\rangle, \tag{A.8}$$

so a "bra-ket" is a "braket". This passes for humor around here.

Linear functions from a vector spaces to $\mathbb{C}$ are also called *dual vectors* or *(linear) functionals*. In the calculus of variation – i.e. the branch of calculus that turns the action principle into the Euler-Langrange equation – the word "functional" is used instead to refer to a function that takes other functions as arguments. Don't be confused by this ambiguity!
In math and engineering, is is common to use a star or sometimes a dagger superscript to denote the functional associated with a vector in a Hilbert space:

$$|\psi\rangle \leftrightarrow \psi, \qquad \langle\psi| \leftrightarrow \psi^* \text{ or } \psi^\dagger.$$

The genius of this notation is that one doesn't need to expend any thoughts on concepts like "dual vectors" or "linear functionals" – the formalism almost forces one to use these object correctly.

Let's play around with this. Equation (A.8) is the *inner product* between $|\psi\rangle$ and $|\phi\rangle$. One can combine two vectors also to form an *outer product*, namely the linear operator $\mathcal{H} \to \mathcal{H}$ defined as

$$|\beta\rangle \mapsto |\phi\rangle\langle\psi|\left(|\beta\rangle\right) := |\phi\rangle\left(\langle\psi|\beta\rangle\right). \tag{A.9}$$

Definition (A.9) implies that composing bra's and ket's is associative: One can read the expression

$$|\phi\rangle\langle\psi|\beta\rangle$$

as either

$$\left(|\phi\rangle\langle\psi|\right)\left(|\beta\rangle\right) \qquad \text{"operator acting on vector"}$$

or as

$$|\phi\rangle\left(\langle\psi|\beta\rangle\right) \qquad \text{"vector times inner product"},$$

getting the same result.

A.1.3 Bases

Let $\mathcal{H}$ be a Hilbert space. A set $\{|e_i\rangle\}_i \subset \mathcal{H}$ is called *ortho-normal* if

$$\langle e_i|e_j\rangle = \delta_{i,j}.$$

If in addition, every element $|\psi\rangle \in \mathcal{H}$ can be expressed as a liner combination

$$|\psi\rangle = \sum_i \psi_i |e_i\rangle$$

with suitable *expansion coefficients* $\psi_i \in \mathbb{C}$, then we have an *ortho-normal basis* (ONB).

> In physics, unless stated otherwise, "basis" always means "ortho-normal basis". Also, one usually assumes that every Hilbert space comes with some distinguished basis. Neither convention is observed in mathematics.

Every ONB fulfills the *completness relation*

$$\sum_i |e_i\rangle\langle e_i| = \mathbb{1}, \tag{A.10}$$

where $\mathbb{1} : |\psi\rangle \mapsto |\psi\rangle$ is the identity map. Prove it!

> The converse is *not* true: There are complete sets that are not ortho-normal bases. A physically important example are the set of coherent states $\{|\alpha\rangle \,|\, \alpha \in \mathbb{C}\}$.

Using just the completeness relation, the following important properties of ONBs can be easily verified:

1. Expansion coefficients are given by inner products

$$|\psi\rangle = \mathbb{1}|\psi\rangle = \Big(\sum_i |e_i\rangle\langle e_i|\Big)|\psi\rangle = \sum_i \underbrace{\langle e_i|\psi\rangle}_{\psi_i} |e_i\rangle.$$

2. Analogous formula for bras:

$$\langle\psi| = \sum_i \underbrace{\langle\psi|e_i}_{\bar{\psi}_i} \, |e_i\rangle.$$

3. Inner products with respect to an arbitrary ONB:

$$\langle\psi|\phi\rangle = \langle\psi|\mathbb{1}|\phi\rangle = \sum_i \langle\psi|e_i\rangle\langle e_i|\phi\rangle = \sum_i \bar{\psi}_i\phi_i.$$

4. Special case of the avove (sometimes called *Parseval relation*):

$$\langle\psi|\psi\rangle = \sum_i |\psi_i|^2.$$

5. Description of operators via *matrix elements*

$$A = \mathbb{1}A\mathbb{1} = \sum_{i,j} |e_i\rangle\langle e_i|A|e_j\rangle\langle e_j| = \sum_{i,j} A_{i,j}|e_i\rangle\langle e_j|, \qquad A_{i,j} := \langle e_i|A|e_j\rangle. \tag{A.11}$$

The Dirac notation allows one to save a bit of ink when working with one fixed ONB. Say we have agreed to work with $\{|e_i\rangle\}_i$. Then quantum physicists (and no-one else...) commonly drop the symbol e and just put the index into the ket:

$$|i\rangle := |e_i\rangle.$$

This shorthand notation can sometimes lead to confusion, but probably offers slightly more advantages than disadvantages. In fact, we'll start using it from now on.

Vector and matrix representations: Assume that $\mathcal{H}$ is finite-dimensional and that some ONB $\{|i\rangle\}_{i=1}^d$ has been fixed. We can then identify the Hilbert space $\mathcal{H}$ with $\mathbb{C}^d$, the set of complex column vectors of size d by mapping an element $|\alpha\rangle \in \mathcal{H}$ to the vector of its expansion coefficients:

$$|\alpha\rangle \mapsto \begin{pmatrix} \alpha_1 \\ \vdots \\ \alpha_d \end{pmatrix}.$$

Such column vectors are particularly useful for computer calculations. Bras, in turn, are mapped to *row* vectors with conjugate coefficients: If

$$|\beta\rangle = \sum_{i=1}^d \beta_i |e_i\rangle,$$

then

$$\langle\beta| = \sum_{i=1}^d \bar{\beta}_i \langle e_i| \mapsto (\bar{\beta}_1, \ldots, \bar{\beta}_d).$$

The usual rules of matrix multpiplication then give

$$(\bar{\beta}_1, \ldots, \bar{\beta}_d) \begin{pmatrix} \alpha_1 \\ \vdots \\ \alpha_d \end{pmatrix} = \sum_{i=1}^d \bar{\beta}_i \alpha_i = \langle\beta|\alpha\rangle,$$

so the two picture are compatible. Likewise, we can map an operator A to the $d \times d$ matrix with elements $A_{i,j} = \langle i|A|j\rangle$. Applying two completeness relations to

$$|\beta\rangle = A|\alpha\rangle \tag{A.12}$$

gives

$$\sum_i |i\rangle\beta_i = \sum_{i,j} |i\rangle A_{i,j}\alpha_j$$

which is equivalent to

$$\begin{pmatrix} \beta_1 \\ \vdots \\ \beta_d \end{pmatrix} = \begin{pmatrix} A_{1,1} & \ldots & A_{1,d} \\ \vdots & & \vdots \\ A_{d,1} & \ldots & A_{d,d} \end{pmatrix} \begin{pmatrix} \alpha_1 \\ \vdots \\ \alpha_d \end{pmatrix}. \tag{A.13}$$

Thus (A.12) and (A.13) link the brak-ket and the matrix picture of the action of operators.

A.1.4 Non-normalizable functions and distributions

When working with function spaces, it makes sense to widen the discourse by allowing for certain generalizations of proper, normalizable functions.

The first example is the set of *plane waves*

$$\phi_{\vec{k}}(\vec{x}) = (2\pi)^{-n/2} e^{i\vec{k}\vec{x}} \tag{A.14}$$

for $\vec{k}, \vec{x} \in \mathbb{R}^n$. These are well-defined functions, but not elements of $L^2(\mathbb{R}^n)$, as their norm is clearly infinite.

More confusion is typically caused by the *Dirac* or *delta distributions* $\delta_{\vec{x}}$. For now, these are just formal elements that we add to the vector space $L^2(\mathbb{R}^n)$. To work with them, *define* the integral of a delta distribution times a *smooth* function ϕ to be

$$\int_{\mathbb{R}^n} \delta_{\vec{x}}(\vec{y})\phi(\vec{y})\,\mathrm{d}^n\vec{y} := \phi(\vec{x}), \qquad \text{and thus} \qquad \langle\vec{x}|\phi\rangle := \langle\delta_{\vec{x}}|\phi\rangle = \phi(\vec{x}). \tag{A.15}$$

One big advantage of adding delta distributions to our framework is that they allow us to formally diagonalize e.g. the position operator

$$(X_i\psi)(\vec{x}) = x_i\,\psi(\vec{x})$$

that does not have any eigenvectors in $L^2(\mathbb{R}^n)$ (why not?). Indeed, the expression

$$X_i = \int |\vec{x}\rangle\, x_i\, \langle\vec{x}|\,\mathrm{d}^n\vec{x}$$

gives the right answer when integrated against smooth functions ψ, ϕ:

$$\begin{aligned}\left\langle\phi\middle|\int x_i|\vec{x}\rangle\langle\vec{x}|\,\mathrm{d}^n\vec{x}\middle|\psi\right\rangle &= \int \langle\phi|\vec{x}\rangle\, x_i\, \langle\vec{x}|\psi\rangle \mathrm{d}^n\vec{x} \\ &= \int \phi^*(\vec{x})\, x_i\, \psi(\vec{x})\,\mathrm{d}^n\vec{x} \\ &= \langle\phi|X_i|\psi\rangle. \end{aligned} \tag{A.16}$$

Neat.

> Delta distributions are often the first concept that is used extensively in physics, but not covered rigorously in the basic analysis courses. They are known to cause a lot of confusion, doubt, and even bouts of disillusionment ("You lured my into physics with the promise of a rigorous understanding of the world – and now you pretent these things are functions when most certainly, they are not! How can I ever trust you again?"). If you feel like this, save your anger.
>
> The first reason is that it is not very difficult to set up a mathematically watertight theory of distributions. For example in terms of *tempered distributions acting on Schwartz space*. There you go. Check out any textbook on functional analysis. In reality, while it's nice to know that functional analysis has your back, practicing researchers don't think about Schwartz space a lot. Instead, they have built a direct intuition for these objects (as will you!). Compare this to the more familiar case of the real numbers. The concept of *irrationality* also once caused confusion, doubt, and even death (to Hippasus, the legend goes,

> drowned by the Gods for realizing $\sqrt{2} \neq r/s$). Today it's easy-peasy to construct the real numbers as simple equivalence classes of converging sequences of rationals. Again, it's good to know that you can rely on the firepower of rigorous arithmetic, but in everyday life, you think of real numbers as points on a line, not as a norm completion via Cauchy sequences.
>
> The second reason why you should save your anger is *that you will actually need it later*! Significant parts of physics *are* built on mathematical dubiousities. So if you continue to cry wolf over distributions, nobody will be there to comfort you after your first encounter with path integrals.

So how, in practice, should one deal with distributions that pop up in equations? Some strategies:

1. *Integrate against smooth functions*. As in (A.16), even if the intermediate mathematical expression contains δ's, they should have all vanished after one has integrated the expression over smooth functions in order to extract physical quantities.

2. *Think of δ is an idealization of "highly concentrated"*. One can in principle replace $\delta_{\vec{x}}$ by functions $\delta_{\vec{x}}^{(\epsilon)}$ that are supported on an ϵ-ball around $\vec{x}$, where ϵ is much smaller than any relevant length scale. The final physical results should then only weakly depend on the actual choice of ϵ, and one should, in fact, be able to take a limit $\epsilon \to 0$. (Physically, the $\delta_{\vec{x}}^{(\epsilon)}$ often make more sense than the idealized $\delta_{\vec{x}}$ – but it is clumsier to work with them, and since ϵ is anyway eliminated in the final step, why bother?)

3. *Shut-up-and-calculate*. The reason δ's are so ubiquitous is that they work well as a computational tool. (A case of *survivor bias*: if the formalism had caused problems, it would have long been abandoned. So the fact alone that it's still around proves that it has non-trivial utility). So in *reality*, people just use them whenever they would have used a Kronecker delta in a finite-dimensional analogue, and pretend that all algebraic manipulations that are valid for Kronecker deltas also extend to distributions. This *mostly* works.

Completeness relation: In the spirit of the third point of view above, we can ask whether the generalization

$$\int |\vec{x}\rangle\langle\vec{x}| \, \mathrm{d}^n\vec{x} = \mathbb{1} \tag{A.17}$$

of the completeness relation (A.10) to the continuous set $\{|\vec{x}\rangle\}_{\vec{x}\in\mathbb{R}^n}$ makes sense. We try the first approach above: For smooth functions ϕ, ψ, the same calculation as in (A.16) confirms that

$$\left\langle \phi \middle| \int |\vec{x}\rangle\langle\vec{x}| \, \mathrm{d}^n\vec{x} \middle| \psi \right\rangle = \langle\phi|\psi\rangle, \tag{A.18}$$

so we accept (A.17) in that sense.

Maybe even more important is the "momentum space" version of (A.18). Recall that the Fourier transform of a function ψ is

$$\tilde{\psi}(\vec{k}) = (2\pi)^{-n/2} \int \psi(\vec{x}) e^{-i\vec{k}\vec{x}} \, \mathrm{d}^n\vec{x} = \langle\vec{k}|\psi\rangle, \tag{A.19}$$

with $|\vec{k}\rangle = |\phi_{\vec{k}}\rangle$ as in (A.14). *Parseval's theorem* from harmonic analysis says that

$$\int \tilde{\phi}(\vec{k})^* \tilde{\psi}(\vec{k}) \mathrm{d}^n \vec{k} = \int \phi(\vec{x})^* \psi(\vec{x}) \mathrm{d}^n \vec{x}. \tag{A.20}$$

Thus

$$\int \tilde{\phi}(\vec{k})^* \tilde{\psi}(\vec{k}) \mathrm{d}^n \vec{k} = \left\langle \phi \middle| \int |\vec{k}\rangle\langle\vec{k}| \, \mathrm{d}^n \vec{k} \middle| \psi \right\rangle = \langle \phi | \psi \rangle$$

so that we conclude that, in the above sense,

$$\int |\vec{k}\rangle\langle\vec{k}| \, \mathrm{d}^n \vec{k} = \mathbb{1}. \tag{A.21}$$

In QM, it makes sense to use the momentum $\hbar\vec{k}$ instead of the wave vector $\vec{k}$ to parameterize plane waves. Remember to include the Jacobian determinant when transforming the integral (A.21) to the coordinates $\vec{p} = \hbar\vec{k}$! Thus, if we set $|\vec{p}\rangle := |\hbar\vec{k}\rangle$, the completeness relation in terms of momenta reads

$$\int |\vec{p}\rangle\langle\vec{p}| \, \frac{\mathrm{d}^n \vec{p}}{\hbar^n} = \mathbb{1}. \tag{A.22}$$

(Alternatively, one can absorb the normalization constant into the definition of the basis vector by setting $|\vec{p}\rangle = \hbar^{-1/2}|\vec{k}\rangle$ for $\vec{k} = \vec{p}/\hbar$.) The lesson here is that in the continuous case, changing the labelling of the vectors might imply a change of the integration measure in the completeness relation. To avoid such nuisances, we will only work with the wave vector parameterization in these notes.

Orthogonality relations: In general, the completeness relation is closely related to a suitable *orthonormality relation*. Let $\{|\lambda\rangle\}$ be any set of vectors that fullfills the completeness relation

$$\int |\lambda\rangle\langle\lambda| \, \rho(\lambda) \, \mathrm{d}\lambda = \mathbb{1} \tag{A.23}$$

with respect to some measure ρ. Then $\mathbb{1}^2 = \mathbb{1}$ implies

$$\int_\lambda \int_{\lambda'} |\lambda\rangle\langle\lambda|\lambda'\rangle\langle\lambda'| \, \rho(\lambda)\mathrm{d}\lambda \, \rho(\lambda')\mathrm{d}\lambda' = \int_\lambda |\lambda\rangle\langle\lambda| \, \rho(\lambda)\mathrm{d}\mu(\lambda)$$

and thus we have the orthogonality relation

$$\langle\lambda|\lambda'\rangle = \frac{\delta(\lambda - \lambda')}{\rho(\lambda)}. \tag{A.24}$$

If $\{|\lambda\rangle\}$ is complete in the sense that it spans the entire Hilbert space, then, conversely, (A.24) implies (A.23).

Spectral measures: TBD.

Operator representations: We can apply the completeness relation for the position basis $\{|\vec{x}\rangle\}$ to operators. This gives a continuous analogue

$$A = \int\int A(\vec{y},\vec{z})\,|\vec{y}\rangle\langle\vec{z}|\mathrm{d}^n y\mathrm{d}^n z, \qquad A(\vec{y},\vec{z}) = \langle\vec{y}|A|\vec{z}\rangle \tag{A.25}$$

of the matrix elements in (A.11). (The function $A(\vec{y},\vec{z})$ specifying the "continuous matrix elements" is sometimes called an *integral kernel*.)

For example, applying (A.25) to the potential operator

$$(V\psi)(\vec{x}) = v(\vec{x})\psi(\vec{x}),$$

associated with a potential $v : \mathbb{R}^n \to \mathbb{R}$ gives

$$V = \int v(\vec{x})\,|\vec{x}\rangle\langle\vec{x}|\mathrm{d}^n\vec{x},$$

as one would expect. If we define (A.25) with respect to the Fourier basis $\{|\vec{k}\rangle\}_{\vec{k}}$ and apply it to the momentum operator $P = -i\hbar\vec{\nabla}$, then

$$\begin{aligned} P(\vec{k},\vec{k}') &= -i\hbar\langle\vec{k}|\vec{\nabla}|\vec{k}'\rangle \\ &= \frac{-i\hbar}{(2\pi)^n}\int e^{-i\vec{k}\vec{x}}\vec{\nabla}e^{i\vec{k}'\vec{x}}\,\mathrm{d}^n\vec{x} \\ &= \frac{\hbar\vec{k}}{(2\pi)^n}\int e^{-i(\vec{k}-\vec{k}')\vec{x}}\,\mathrm{d}^n\vec{x} \\ &= \hbar\vec{k} \end{aligned}$$

and thus

$$P = \int \hbar\vec{k}\,|\vec{k}\rangle\langle\vec{k}|\,\mathrm{d}^n\vec{k},$$

also to nobody's surprise.

We really should stop while we're ahead – but instead, let's get adventurous and represent the momentum operator in *position* basis (for $n = 1$, to keep things simpler):

$$\langle y|P|z\rangle = -i\hbar\int \delta_y(x)\partial_x\delta_z(x)\,\mathrm{d}x = -i\hbar\int \delta_y(x)\delta_z'(x)\,\mathrm{d}x = -i\hbar\delta_z'(y).$$

The result is a "distribution-valued integral kernel" and a formal expression

$$P = \int\int |y\rangle\, i\hbar\delta_y'(z)\,\langle z|\,\mathrm{d}y\mathrm{d}z$$

for the momentum operator. Amazingly, one can make sense of this! Integrating against smooth functions ϕ, ψ that vanish at infinity (so that we can use integration by parts to "shift the derrivative" to the other factor in the integral):

$$\begin{aligned} \int\int \phi(y)^*\ (i\hbar)\delta_y'(z)\,\psi(z)\,\mathrm{d}y\mathrm{d}z &= -\int\int \phi(y)^*\ (i\hbar)\delta_y(z)\,\psi'(z)\,\mathrm{d}y\mathrm{d}z \\ &= -i\hbar\int \phi(y)^*\,\psi'(y)\mathrm{d}y = \langle\phi|P|\psi\rangle. \end{aligned}$$

The formulas

$$P = -i\hbar\int |\delta_x\rangle\langle\delta_x'|\,\mathrm{d}^n x \qquad \text{and} \qquad P = -i\hbar\int |x\rangle\partial_x\langle x|\,\mathrm{d}x \tag{A.26}$$

make sense in the same way.

Quantization in a finite volume: Imaging a world in which every function has period L in each coordinate (Fig. **??**). Mathematically, this would be convenient, as the space of periodic functions has a *countable* Fourier basis. Indeed, only wave vectors

$$\vec{k}, \qquad k_i = \frac{n_i}{2\pi L}, \qquad n_i \in \mathbb{Z}$$

with coefficients integer multiples of $(2\pi L)^{-1}$ are compatible with periodicity.

What is more, the "unit cell" $B = [-L/2, L/2] \times [-L/2, L/2] \times [-L/2, L/2]$, a box of side length L centered at the origin, contains all information about the periodic universe. We can therefore restrict attention to the Hilbert space $L^2(B)$ of periodic functions $B \to \mathbb{C}$, with inner products given by integrals over B only. This space is spanned by the Fourier basis

$$\phi_{\vec{k}}(\vec{x}) := \frac{1}{L^{n/2}} e^{i\vec{k}\vec{x}}, \qquad k \in \mathbb{Z}^3/(2\pi L),$$

which now consists of proper, normalizable functions

$$\int_B \phi^*_{\vec{k}}(\vec{x}) \phi_{\vec{k}'}(\vec{x}) \, \mathrm{d}^3\vec{x} = \delta_{\vec{k},\vec{k}'}.$$

The formulas for the Fourier transform become

$$\begin{aligned} \tilde{f}(\vec{k}) &= \frac{1}{L^{3/2}} \int_B e^{-i\vec{k}\vec{x}} f(\vec{x}) \, \mathrm{d}^3\vec{x}, \\ f(\vec{x}) &= \frac{1}{L^{3/2}} \sum_{\vec{k} \in \mathbb{Z}^3/(2\pi L)} \tilde{f}(\vec{k}) e^{i\vec{k}\vec{x}}. \end{aligned}$$

Comparison with (A.19) shows that, formally, the transition between a finite and an unbounded volume is facilitated by the substitution

$$\frac{1}{\pi^{3/2}} \int_{\mathbb{R}^3} \mathrm{d}^3\vec{k} \quad \leftrightarrow \quad \frac{1}{L^{3/2}} \sum_{\vec{k} \in \mathbb{Z}^3/(2\pi L)} . \tag{A.27}$$

While having a discrete, normalizable Fourier basis might be mathematically desirable, there is the minor issue that the world isn't actually periodic... ...but we might as well pretend it were! Physics is local, so we may assume that all phenomena we are interested in take place in some box that is sufficiently large that the boundary does not affect the predictions we extract from the theory. In this sense, expressions that ony differ from one another by the substitution (A.27) should be thought of as having the same physical content. Which one is employed is purely a function of mathematical convenience, and authors are known to switch between them without further comment.

Attention! Sometimes, one restricts to compact regions to model a *physical* boundary affecting the system: e.g. to describe a particle trapped in a box, or EM radiation propagating in a wave guide with conducting boundary. These physical constraints should not be confused with the ones we adopt merely for mathematical convenience.

A.1.5 A zoology of operators

Let A be an operator on $\mathcal{H}$. There is a unique operator $A^\dagger$ which fulfills

$$\langle \psi | A\phi \rangle = \langle A^\dagger \psi | \phi \rangle \qquad \forall \psi, \phi \in \mathcal{H}$$

(why?). One can easily verify:

$$A = \sum_{i,j} A_{i,j} |i\rangle\langle j| \qquad \Leftrightarrow \qquad A^\dagger = \sum_{i,j} \overline{A_{j,i}} |i\rangle\langle j|,$$

so that, in the matrix picture, the adjoint corresponds to the combination of the transpose and the complex conjugation. A useful consequence is

$$\left(z\,|\psi\rangle\langle\phi|\right)^\dagger = \overline{z}|\phi\rangle\langle\psi|. \tag{A.28}$$

An operator A is *self-adjoint* (or *Hermitian*) if $A = A^\dagger$. As *observables*, self-adjoint operators play, of course, an important role in quantum mechanics. There are a number of equivalent characterizations of self-adjointness:

1. $A = A^\dagger$.
2. For all $\psi, \phi \in \mathcal{H}$, it holds that $\langle\psi|A|\phi\rangle = \overline{\langle\phi|A|\psi\rangle}$. In particular, the matrix representation of A w.r.t. any ONB is invariant under taking the transpose and the complex conjugate.
3. The operator A has an ortho-normal eigenbasis and real eigenvalues:

$$A = \sum_i \lambda_i |f_i\rangle\langle f_i|, \qquad \lambda_i \in \mathbb{R}, \quad \langle f_i|f_j\rangle = \delta_{i,j}.$$

Proof. Exercise. □

An operator P is called a *projection* if it squares to itself $P^2 = P$ and is self-adjoint $P = P^\dagger$.

> Outside of QM, the term *projection* often just means "squares to itself". Operators that square to themself and are also Hermitian are then called *orthogonal projections*. In QM, the adjective "orthogonal" is usually implied, as non-orthogonal projections rarely occur (to the extend that I have seen experienced physicsts being surprised when realizing that such objects do exist).

These are equivalent:

1. P is a projection.
2. P is Hermitian and all eigenvalues are equal to either 0 or 1.
3. There is a set $\{|f_i\rangle\}_{i=1}^r$ of ortho-normal vectors such that

$$P = \sum_{i=1}^r |f_i\rangle\langle f_i|$$

Proof. Exercise. □

An operator U is called *unitary* if it preserves inner products:

$$\langle U\psi|U\phi\rangle = \langle\psi|\phi\rangle, \qquad \forall\, \psi, \phi \in \mathcal{H}.$$

These are equivalent for an operator U:

1. U is unitary.
2. $U^\dagger = U^{-1}$.
3. U preserves lengths:

$$\|U\psi\| = \|\psi\| \qquad \forall \psi \in \mathcal{H} \tag{A.29}$$

4. U has an ortho-normal eigenbasis and eigenvalues of absolut value 1:

$$U = \sum_j e^{i\phi_j} |f_j\rangle\langle f_j|, \qquad \langle f_i|f_j\rangle = \delta_{i,j}, \quad \phi_j \in \mathbb{R}$$

5. There is a self-adjoint operator H such that

$$U = e^{iH}. \tag{A.30}$$

The final formlation links quantum mechanical time evolutions to Hamiltonians. Unitaries are exactly the *linear* isometries of the Hilbert space. Anti-linear isometries also play an important role – we'll encounter them later.

A.2 Modelling a quantum experiment

Quantum mechanics makes probabilistic predictions about the outcome of physical experiments. To extract predictions from the theory, one first needs to *model* the physical setup mathematically.

In the simplest caset, one associates these objects with every quantum system:

1. A *Hilbert space* $\mathcal{H}$. Like the phase space in Hamiltonian mechanics, this is the central object of the theory.
2. A Hermitian operator H acting on $\mathcal{H}$. This is the *Hamiltonian* which determines the time evolution of the system, if it is isolated from the environment.

What is more:

3. With every *preparation procedure* of the system, one associates a *state*. An important class are *pure states* that are described by unit-length vectors $|\psi\rangle \in \mathcal{H}$.
4. Finally, we need to describe *measurements* on the system. The easiest class of measurements are associated with a Hermitian operator, called an *observable*.

The *axioms of quantum mechanics* then tell us how to extract predictions from this data.

Specifically, assume we prepare a system in an initial state $|\psi(0)\rangle$; let it evolve for time t under its Hamiltonian H; and finally measure an observable A.

The time evolution of the state is given the *time evolution operator* $U(t)$:

$$|\psi(t)\rangle = U(t)|\psi(0)\rangle, \qquad U(t) = e^{\frac{1}{i\hbar}tH} = \sum_{k=0}^{\infty} \frac{1}{k!} \left(\frac{t}{i\hbar}\right)^k H^k.$$

Equivalently, the state satisfies the *Schrödinger equation*

$$i\hbar\partial_t|\psi(t)\rangle = H|\psi(t)\rangle.$$

The measurement is described in terms of the eigendecomposition

$$A = \sum_i \lambda_i |f_i\rangle\langle f_i|$$

of the observable. The (simplest form of the) measurement axiom says that the experiment will yield the i-th outcome with probability

$$p_i = |\langle\psi(t)|f_i\rangle|^2.$$

The eigenvalue λ_i is a numerical constant we associate with the i-th outcome. Often, this rule is stated in terms of the *expectation value*

$$\begin{aligned}\langle A\rangle :=& \sum_i \lambda_i p_i = \sum_i \lambda_i \langle\psi(t)|f_i\rangle\langle f_i|\psi(t)\rangle = \langle\psi(t)|\Big(\sum_i \lambda_i |f_i\rangle\langle f_i|\Big)|\psi(t)\rangle \\ =& \langle\psi(t)|A|\psi(t)\rangle.\end{aligned}$$

While the formulation presented above is enough for most elementary applications, it is not general enough to describe all physically relevant situations.

In practice, preparation schemes do not give pure states (described by Hilbert space vectors), but *mixed states* associated with *density matrices*. Systems are not isolated, but *open*, i.e. interacting with an uncontrolled environment. The time evolution is then described by a *completely positive map* rather than a unitary time evolution operator. Not all measurements are described by observables. In the most general framework, measurements are associated with so-called *positive operator-valued measures (POVMs)*.

The data $\mathcal{H}, H$ that goes into the definition of the theory is not, in general, complete. One sometimes adds *super selection rules* that specify a subset of states and/or observables that are considered physical. For example, we explain in Sec. **??** that observables for many-Fermion systems are required to be polynomials of *even order* in the ladder operators.

A.3 Fermi's golden rule

We recall the derivation of *Fermi's golden rule*, a standard method from time-dependent perturbation theory.

Consider a family of Hamiltonians

$$H(\lambda) = H_0 + \lambda V.$$

Denote the eigenstates of the unperturbed Hamiltonian H_0 as $\{|n\rangle\}_n$. Assume that $\langle n|V|n\rangle = 0$. For any fixed λ, let $|\psi(t,\lambda)\rangle$ be the solution of the Schrödinger equation. As is standard in quantum mechanical perturbation theory, we assume (without much in the way of proof) that one can exapnd

$$|\psi(t,\lambda)\rangle = \sum_{s=0}^{\infty} \lambda^s |\psi_s(t)\rangle$$

as a power series in λ and that low orders give meaningful answers. Seperating the Schrödinger equation

$$i\hbar\partial_t\Big(\sum_s \lambda^s|\psi_s\rangle\Big) = (H_0+\lambda V)\Big(\sum_s \lambda^s|\psi_s\rangle\Big)$$

by degrees of λ gives

$$\begin{aligned} i\hbar\partial_t|\psi_0\rangle &= H_0|\psi_0\rangle && \text{0th order}\\ i\hbar\partial_t|\psi_1\rangle &= H_0|\psi_1\rangle + V|\psi_0\rangle && \text{1st order}\\ &\vdots && \vdots \end{aligned}$$

With initial condition

$$|\psi(t=0)\rangle = |i\rangle,$$

The zeroth-order equation is solved by

$$|\psi_0(t)\rangle = e^{\frac{t}{i\hbar}E_i}|i\rangle.$$

Plugging this into the first-order one and projecting onto $|f\rangle$ gives

$$i\hbar\partial_t\langle f|\psi_1(t)\rangle = E_f\langle f|\psi_1(t)\rangle + e^{\frac{t}{i\hbar}E_i}\underbrace{\langle f|V|i\rangle}_{=:g_f}$$

solved by

$$\langle f|\psi_1(t)\rangle = g_f\frac{1-e^{\frac{1}{i\hbar}(E_i-E_f)t}}{E_f-E_i}e^{\frac{1}{i\hbar}E_ft} \qquad \text{for} \quad E_f\neq E_i, \tag{A.31}$$

$$\langle f|\psi_1(t)\rangle = g_f\frac{t}{i\hbar}e^{\frac{1}{i\hbar}E_ft} \qquad \text{for} \quad E_f=E_i, f\neq i, \tag{A.32}$$

$$\langle f|\psi_1(t)\rangle = 0\frac{t}{i\hbar}e^{\frac{1}{i\hbar}E_it} \qquad \text{for} \quad f=i.$$

(Using L'Hôspital's rule, one verifies that (A.31) tends to (A.32) for $E_f\to E_i$).

The squares are

$$|\langle f|\psi(t)\rangle|^2 = |g_f|^2\frac{2(1-\cos(\frac{1}{\hbar}(E_i-E_f)t))}{(E_i-E_f)^2} = |g_f|^2\frac{4\sin^2((E_i-E_f)\frac{t}{2\hbar})}{(E_i-E_f)^2}, \quad E_i\neq E_f$$

$$|\langle f|\psi(t)\rangle|^2 = |g_f|^2\frac{t^2}{\hbar^2} \qquad E_i=E_f,$$

$$|\langle i|\psi(t)\rangle|^2 = 1.$$

Clearly, normalization is *not* preserved. Thus, first-order perturbation theory must break down at least once a considerable amount of weight has been transferred away from $|i\rangle$. We'll come back to this. (It is not actually surprising that the *increase* of weight on previously unoccupied levels shows up in lower order perturbation theory than the decrease of weight on the initial level – Fig. **??**).

With $\epsilon = (E_i-E_f)$, $\tau = \frac{t}{2\hbar}$, the fraction is $\sin^2(\epsilon\tau)/\epsilon^2$, the square of the "sinc function" (Fig. **??**). It has a central peak of height τ, zeroes at $\epsilon = \pm\frac{\pi}{\tau}$, and shows

oscillations of quadratically decreasing amplitude for $\epsilon \to \pm\infty$. It is known (by the *Dirichlet integral*) that the area under the curve is $\tau\pi$.

This indicates that only states with energies in the range $\pm\frac{\pi}{\tau}$ pick up significant weight. Assume that in this range, the energy levels of H_0 are roughly evenly spaced, with gaps much smaller than the interval length, and with a density of $n(E_i)$ states per unit energy. Let's also assume for now that the coupling strength $|g_f|^2 = |g_E|^2$ only depends on the energy. Then

$$\sum_{f\neq i} |\langle f|\psi(t)\rangle|^2 \simeq t \underbrace{\frac{\pi}{2\hbar}|g_{E_i}|^2\, n(E_i)}_{=:\Gamma}\,.$$

Thus, for times long enough that the sinc^2-functions has already concentrated for these approximations to hold, but short enough that first-order perturbation theory hasn't yet broken down, the occupancy of levels with energy $E_f \simeq E_i$ grows linearly in time, with known rate Γ. Using the normalization condition (not directly given by first-order approximation theory, see above),

$$|\langle i|\psi(t)\rangle|^2 = (1 - t\Gamma).$$

We now have to interpolate this situation for larger times. It is not obvious what will happen. If we assume that the process is effectively irreversible, i.e. that no weight flows back to the initial level, then it is plausible that repeating the process for another t time units gives

$$|\langle i|\psi(2t)\rangle|^2 = (1 - t\Gamma)^2$$

and so on. If that is indeed true, we may extrapolate

$$|\langle i|\psi(2t)\rangle|^2 \simeq e^{-t\Gamma}.$$

We note that in this final paragraph, we just appealed to intuition about how a complex system with a very larger number of levels might behave. This is not a proof and not even a well-justified approximation. No simple analysis that would indicate in exactly which regime exponential decay happens is known to me. Still, the calculation often seems to give right results, so let's work with it for now.

Appendix B

Symmetries in quantum mechanics

In Chapter **??**, we will guess a quantum description of relativistic phenomena. What tools do we have available to guide the construction of new theories? The most fundamental and powerful technique is to require that the theory reproduce physical *symmetries*.

B.1 Symmetry groups

It is an empirical fact that the result of physical experiments are independent of *where*, *when*, *in which orientation*, and *at which constant velocity* they are being conducted. In non-relativistic physics, these *space-time symmetries* are described by the *Galileo transformations*

$$\begin{pmatrix} t \\ \vec{x} \end{pmatrix} \mapsto \begin{pmatrix} t+s \\ R\vec{x} + \vec{v}t + \vec{a} \end{pmatrix}$$

with

$\vec{a} \in \mathbb{R}^3$	translation of the spatial origin
$\vec{v} \in \mathbb{R}^3$	uniform velocity
$R \in \mathrm{SO}(3)$	rotation of space
$s \in \mathbb{R}$	offset of origin of time.

These operations can be inverted and composed – in mathematical terms, they form a *group*. We will take this property to be part of the definition of a "symmetry".

Symmetry groups act in various ways on the ingredients of quantum theory (states, observables, wave equations...). Analyzing these actions turns out to be highly fruitful.

B.2 Kinematic symmetries

The action of symmetries on quantum descriptions is easiest for *kinematic symmetries*, which are the ones that leave the time coordinate invariant.

B.2.1 Wigner's Theorem:

Consider the preparation of a state ρ, immediately followed by the measurement of an observable A. The expectation value of the outcome is

$$\langle A\rangle_\rho = \mathrm{tr}\,\rho A.$$

Now choose some kinematic Galileo transformation (Fig. **??**). The displaced preparation procedure will be associated with some state ρ'. Likewise, the displaced measurement is described by some observable A'.

$$\mathrm{tr}\,\rho A = \mathrm{tr}\,\rho' A'. \tag{B.1}$$

What kind of transformations

$$\rho \mapsto \rho', \qquad A \mapsto A'$$

preserve expectation values? The simplest possible class of solutions to (B.1) is given by unitary transformations:

$$\rho' = U\rho U^\dagger, \qquad A' = UAU^\dagger \tag{B.2}$$

for some unitary U. A priori, much more complicated, highly non-linear transformation could also occur. Fortunately, it turns out that the most naive guess (B.2) is essentially all that can happen:
[Wigner's Theorem] *Every symmetry transformation is of the form*

$$\rho' = T\rho T^\dagger, \qquad A' = TAT^\dagger, \tag{B.3}$$

where $T : \mathcal{H} \to \mathcal{H}$ is either unitary or anti-unitary.

[Anti-linear maps] A map T is *anti-linear* if it fulfills

$$T(|\alpha\rangle + |\beta\rangle) = T(|\alpha\rangle) + T(|\beta\rangle), \qquad T(z|\alpha\rangle) = \bar{z}\,T(|\alpha\rangle).$$

An obvious anti-linear map is *complex conjugation* with respect to some basis:

$$C\big(\sum_i c_i|i\rangle\big) = \sum_i \bar{c}_i|i\rangle.$$

Fortunately, it turns out that this is the only example you really have to know about, as any anti-linear T can be written as

$$T = LC \tag{B.4}$$

for some *linear* map L.
Here's the reason: The composition TS of two anti-linear maps T, S is linear:

$$T\big(S(z|\alpha\rangle)\big) = T\big(\bar{z}S(|\alpha\rangle)\big) = zTS|\alpha\rangle.$$

Thus, using $CC = \mathbb{1}$,

$$T = TCC = LC, \qquad L := TC.$$

The *adjoint* of an anti-linear map is defined by requiring

$$\langle T^\dagger\psi|\phi\rangle = \langle\psi|T\phi\rangle^* \qquad \forall\psi,\phi.$$

Writing $T = LC$,

$$\langle\psi|LC\phi\rangle^* = \langle L^\dagger\psi|C\phi\rangle^* = \langle CL^\dagger\psi|\phi\rangle = \langle L^T C\psi|\phi\rangle,$$

so that $T^\dagger = L^T C$.

A map T is *anti-unitary* if TC is unitary. By the above, demanding that T be unitary or anti-unitary is equivalent to demanding $T^\dagger T = \mathbb{1}$.

There is no continuous function $\lambda \mapsto T_\lambda$ such that T_λ is unitary for some values of λ and anti-unitary for other values of λ. That's because

$$T(i\mathbb{1})T^\dagger = +i\mathbb{1} \qquad \text{for all unitary } T$$
$$T(i\mathbb{1})T^\dagger = -i\mathbb{1} \qquad \text{for all anti-unitary } T,$$

and clearly, there's no way to continuously change the two right-hand sides into each other.

The final remark above implies that any symmetry transformation that can be contiuously connected to the identity has to be unitary. It turns out that in the context of space-time symmetries, only those that reverse the flow of time are anti-linear.

[On the proof of Wigner's Theorem] The usual (and original) formulation of Wigner's Theorem is this: Let $T : \mathcal{H} \to \mathcal{H}$ be a map that preserves the squared inner product.

$$|\langle\phi|\psi\rangle|^2 = |\langle T(\phi)|T(\psi)\rangle|^2. \tag{B.5}$$

Then T is either *unitary* or *anti-unitary*.

The proof doesn't use advanced math, but is remarkably tedious. Various versions can be found e.g. in [Weinberg, Arkadi, Cassinelli]. (It is related to the *Fundamental Theorem of Projective Geometry*).

In the literature (and in Wigner's original work) it is usually postulated that any symmetry transformation must act on Hilbert space vectors (rather than density matrices and observables) and must satisfy (B.5). Our starting point – Eq. (B.1) – assumes a bit less. To connect it to (B.5), one has to establish two statements: First, symmetries map pure states $\rho = |\psi\rangle\langle\psi|$ to pure states, and rank-one observables $A = |\phi\rangle\langle\phi|$ to rank-one observables. One can therefore express the action on operators in terms of the action on Hilbert space vectors. Second, the map acting on vectors comming from states is the same as the map on vectors coming from observables. Neither statement is difficult to prove. The details – and much more! – can be found in the excellent (if somewhat technical) book [Cassinelli].

[Compatibility with time evolution] A symmetry acts on observables as $A \mapsto A' = TAT^\dagger$. The Hamiltonian H has two functions: As an observable, it describes energy measurements. But it is also the generator of time evolution: $U(t) = e^{-itH}$.

It could be that the "Hamiltonian-as-generator" transforms differently from the "Hamiltonian-as-observable". Fortunately, that's not the case. To see this, consider an experiment where we let the state evolve for some time τ between preparation and measurement. Then

$$\begin{aligned}\mathrm{tr}\left(e^{-i\tau H}\rho e^{i\tau H}A\right) &= \mathrm{tr}\left(Te^{-i\tau H}T^\dagger T\rho T^\dagger Te^{i\tau H}T^\dagger TAT^\dagger\right)\\ &= \mathrm{tr}\left(e^{-i\tau THT^\dagger}T\rho T^\dagger e^{i\tau THT^\dagger}TAT^\dagger\right)\\ &= \mathrm{tr}\left(e^{-i\tau H'}\rho' e^{i\tau H'}A'\right)\end{aligned} \tag{B.6}$$

having used the fact that a real-valued trace is invariant under conjugation by both unitary and anti-unitary maps.

B.2.2 Representations

Let g_1, g_2 be two elements of the symmetry group, with $g = g_2 g_1$ their composition. Displacing physical systems by g can be achieved by first applying g_1 and then g_2 (Fig. **??**). Therefore, $T_{g_1}\, T_{g_2}|\psi\rangle$ and $T_{g_1 g_2}|\psi\rangle$ must describe the same physical state. As two vectors give rise to the same state if and only if they differ by a phase factor, we must have

$$T_{g_1} T_{g_2} = e^{i\lambda(g_1,g_2)} T_{g_1 g_2} \tag{B.7}$$

for some function $\lambda(g_1, g_2) \in \mathbb{R}$.

A correspondence

$$g \mapsto T_g$$

fulfilling (**??**) is called a *projective representation* of the group. If the phase factor is always equal to 1, it is a *linear representation* or just a *representation*. We have thus found:

- The Hilbert space of a quantum system carries a projective unitary or anti-unitary representation of the group of symmetries.

B.2.3 Space-time symmetries

[Somehwat pedantic. May be skipped.]

What about time translation symmetry $(t, \vec{x}) \mapsto (t + s, \vec{x})$ that is part of the Galileo group? The way we have set up the theory, it is *manifestly* invariant under time shifts, *because no absolute time coordinate ever appears*. Only the relative time τ since preparation enters (c.f. Eq. (B.6)). Thus, the action of time translation in our formulation is trivial. The underlying reason is that the acts of "preparation" and "measurement" – thought to be triggered by an external observer – provide temporal reference points.

One usually adds extra assumptions to the effect that the invariance of the theory under general space-time symmetries does not hinge on external preparation and measurement processes. (Note that Wigner's Theorem does not apply in this context any more, as its starting point is the invariance of measurement statistics). We'll discuss two approaches.

Wave functions as fields: Let's ditch the general, high-level reasoning employed so far, and adopt a very down-to-earth assumption: Quantum states and their time evolutions are described by (possibly vector-valued) functions $\psi(t, \vec{x})$ on space-time, which satisfy a linear differential equation

$$D\psi(t, \vec{x}) = 0, \tag{B.8}$$

where D is some expression in the $\partial_t, \partial_{x_i}$ generalizing the Schrödinger equation. One also assumes that the space-time translations $\vec{x}' = \vec{x} + a, t' = t + s$ act by shifting these functions

$$\psi'(t', \vec{x}') = \psi(t' - s, \vec{x}' - a). \tag{B.9}$$

At this point, one does not know how the homogeneous parts of the space-time symmetry group act. But we know that the action has to preserve the solution space (B.8) and

be compatible with translations (B.9). These consistency conditions often massively narrow the possibilities (we'll work through one important case in Chapter 3).

If the wave equation (B.8) is first-order in time, we can write it as

$$i\partial_t \psi = H\psi$$

for some operator H that only depends on spatial derrivatives. Time evolution is then described in the familiar way as

$$\psi(t, \vec{x}) = e^{-itH}\psi(0, \vec{x}). \tag{B.10}$$

In particular, the wave function is fully determined by its values at $t = 0$. Thus, if the full space-time symmetry group acts on wave functions on $\mathbb{R}^4$, we can use (B.10) to define an action only on the time slice at $t = 0$. This is the idea behind the second approach, desribed next.

> One can classify all representations of the Poincaré group (using what physicists call *Wigner's method of the Little Group* and mathematicians refer to as *Mackey's Machine*). It turns out that the physically relevant, non-trivial unitary representations all arise as actions on fields in some sense – so in the relativistic case, the concrete model used here can be motivated from more general considerations [**?**, **?**].
>
> The situation is less clear in the non-relativstic case. Indeed, a single spin-$1/2$ without any spatial degrees of freedom carries a perfectly fine unitary representation of the Galileo group.

Hamiltonian as generator of time shifts: A basic axiom of QM is that time evolution is implemented by unitary maps $U(s) = e^{isH}$. Now time evolution is *not* a symmetry (e.g. it manifestly changes expectation values). However, we can use the existence of the $U(s)$'s to find a description of QM, where the full space-time group is represented on the system's Hilbert space.

The cleanest way of doing this is to pass to *Heisenberg picture*. Consider again a state preparation of $|\psi\rangle$ at time t_0, followed by a measurement of an observable A at time t_1. Define

$$\begin{aligned} |\psi_H\rangle &= e^{it_0 H}|\psi\rangle && \text{“state at time 0”}, \\ A_H &= e^{it_1 H} A e^{-it_1 H} && \text{“observable at time } t_1\text{”}. \end{aligned}$$

(The “H” in ψ_H, A_H is for Heisenberg, not Hamilton). Then the expectation value of the experiment

$$\operatorname{tr} e^{-i(t_1-t_0)H}|\psi\rangle\langle\psi|e^{i(t_1-t_0)H}\, A$$

can be expressed as

$$\operatorname{tr} |\psi_H\rangle\langle\psi_H| A_H.$$

Now if the experiment gets carried out s time units later, then

$$|\psi'_H\rangle\langle\psi'_H| = e^{isH}|\psi_H\rangle\langle\psi_H|e^{-isH}, \qquad A'_H = e^{isH} A_H e^{-isH},$$

so the time shift corresponds to the action of $T = U(-s) = e^{isH}$ on the Heisenberg picture description of states and observables. The kinematic symmetries must also act on these objects, by Wigner's Theorem.

> TBD: Toy theory to show that these are indeed extra assumptions.

B.3 Lie algebras

We have seen that any Hilbert spaces carrise a projective representation of the space-time symmetry group. Since we usually have a pretty good idea of what the symmetries of a system are (e.g. Galileo, Poincaré, ...), but might not know how to decribe the system quantum mechanically, it is a good idea to classify *all* representations. If we are lucky (and we often are), there's only a few and we can check for each whether it leads to a theory reproducing the behavior of the system at hand.

The single most important tool for finding representations of continuous groups is to look at their "infinitesimal generators", also know as their *Lie algebras*.

Let G be a continuous matrix group. Our running example will be

$$G = \mathrm{SO}(3) = \{\text{real } 3 \times 3 \text{ matrices } O \,|\, O^T O = \mathbb{1}\}.$$

Generators from the group: Let $R(t)$ be a path in G, with $R(0) = \mathbb{1}$ (Fig. **??**). Expanding each matrix elements in t gives

$$R(t) = \mathbb{1} + tM + O(t^2)$$

for some matrix M. One refers to the M's arising this way as the *generators* of G. Sometimes, for "small t", one uses the less preicse term *infinitesimal transformation* for $\mathbb{1} + tM$. Geometrically, M is a tangent vector to G at $\mathbb{1}$ (see figure). The set of generators is called the *Lie algebra* of G and denoted as $\mathrm{Lie}(G)$.

Group from the generators: Let M be a generator. Then it turns out that

$$R(t) := e^{tM} = \mathbb{1} + tM + \frac{t^2}{2}M^2 + \dots$$

is an element of the group. What is more, *all* elements of G that are "sufficiently close" to $\mathbb{1}$ arise this way. In fact, in all cases relevant to us, every group element that can be continuously connected to $\mathbb{1}$ at all, can be expressed by exponentiating a generator. These statements are at the heart of Lie theory and will not be proven here.

The two most important properties of the Lie algebra are these:

1. $\mathrm{Lie}(G)$ is a vector space.
2. $\mathrm{Lie}(G)$ is closed under taking commutators:

$$M_1, M_2 \in \mathrm{Lie}(G) \;\Rightarrow [M_1, M_2] \in \mathrm{Lie}(G).$$

[Proof sketch.] For the first claim: Set $R(t) = e^{tM_1} e^{tM_2}$. Then

$$\frac{\mathrm{d}}{\mathrm{d}t}\Big|_{t=0} R(t) = M_1 + M_2.$$

For the second: Define

$$R^{(s)}(t) = e^{sM_1} e^{tM_2} e^{-sM_1}.$$

Then for all s it holds that $t \mapsto R^{(s)}(t)$ is a path in G, so that $\frac{\mathrm{d}}{\mathrm{d}t} R^{(s)}(0) \in \mathrm{Lie}(G)$. But because $\mathrm{Lie}(G)$ is a vector space, it contains the tangent vectors to all curves that lie in $\mathrm{Lie}(G)$. Thus

$$\mathrm{Lie}(G) \ni \frac{\mathrm{d}}{\mathrm{d}s}\Big|_{s=0}\Big(\frac{\mathrm{d}}{\mathrm{d}t}\Big|_{t=0} R^{(s)}(t)\Big) = \frac{\mathrm{d}}{\mathrm{d}s}\Big|_{s=0}\Big(e^{sM_1} M_2 e^{-sM_1}\Big) = [M_1, M_2]. \tag{B.11}$$

□

One of the most important questions of the theory is this: We have seen that the commutator of generators is again a generator. But what is the *meaning* of $[M_1, M_2]$? This answer:

- The commutator of generators corresponds to the composition of group elements.

This is made precise by the *Baker-Campbell-Hausdorff formula*

$$e^A e^B = \exp\Big\{A + B + \frac{1}{2}[A,B] + \frac{1}{12}[A,[A,B]] + \underbrace{\cdots}_{\text{further, nested commutators}}\Big\}, \quad \text{(B.12)}$$

for A, B sufficiently small.

> The general proof of the BCH formula is not simple. Historically, it tooks several attempts before an explicit and correct version emerged. For low orders, one can find the commutator expressions in (B.12) by setting $A = t\tilde{A}, B = t\tilde{B}$ and Taylor expanding both sides in t.

Example – The rotation group: TBD.

B.3.1 Representations

By the BCH formula, the group law is encoded in the commutator relations of the generators. It thus plausible that representations of the group are connected to representations of the Lie algebra. This is almost true (and fails in a very interesting way – we'll see).

Group representation → Lie algebra representation: Let $g \mapsto T_g$ be a unitary representation of G. That is, we require

$$T_g \text{ unitary on some Hilbert space } \mathcal{H}, \qquad T_{g_2} T_{g_1} = T_{g_2 g_1}.$$

(We'll treat the projective version below). Consider a generator

$$M = \frac{\mathrm{d}}{\mathrm{d}t}\Big|_0 R(t).$$

Define

$$t(M) := \frac{\mathrm{d}}{\mathrm{d}t}\Big|_0 T(R(t)).$$

Then $M \mapsto t(M)$ defines a *representation of* $\mathrm{Lie}(G)$ in the sense that

1. t is linear:

$$t(M_1 + cM_2) = t(M_1) + ct(M_2).$$

2. t preserves commutators:

$$[t(M_1), t(M_2)] = t([M_1, M_2]).$$

[Proof sketch] The first claim follows just by using the chain and the product rule.
For the second claim:

$$\begin{aligned} t([M_1,M_2]) &= t\Big(\frac{\mathrm{d}}{\mathrm{d}s}\Big|_0 \frac{\mathrm{d}}{\mathrm{d}t}\Big|_0 e^{sM_1}e^{tM_2}e^{-sM_1}\Big) && \text{Eq. (B.11)} \\ &= \frac{\mathrm{d}}{\mathrm{d}s}\Big|_0 t\Big(\frac{\mathrm{d}}{\mathrm{d}t}\Big|_0 e^{sM_1}e^{tM_2}e^{-sM_1}\Big) && \text{linearity of } t \\ &= \frac{\mathrm{d}}{\mathrm{d}s}\Big|_0 \frac{\mathrm{d}}{\mathrm{d}t}\Big|_0 T\Big(e^{sM_1}e^{tM_2}e^{-sM_1}\Big) && \text{definition of } t \\ &= [t(M_1),t(M_2)] && \text{Eq. (B.11).} \end{aligned}$$

Thus, every group representation implies a Lie algebra representation.

Lie algebra representation $\to$ group representation: By the BCH formula, if one can construct matrices that satisfy the same commutator relations as $\mathrm{Lie}(G)$, then exponentiating gives a representation of the group – at least for elements sufficiently close to $\mathbb{1}$. What is even better:

- If a reprsentation of the Lie algebra is irreducible, then by exponentiating it, one obtains a projective representation of the group.

In other words, even if BCH fails to converge for "elements far away from $\mathbb{1}$", the worst that can happen is that phase factors appear. But that's just fine with us: As explained above, we actually look for *projective* representations. Therefore, for the purpose of classifying the action of connected symmetry groups on quantum sysytems, it is enough to find representations of the Lie algbra!

The appearance of phase factors has a fascinating topological origin – see Fig. **??**.

Example – Spin representations:

B.3.2 Central extensions

We have seen that when passing from commutator relations to the symmetry group, then phase factors might appear for elements "far away from $\mathbb{1}$". More generally, there are projective representations that manifest themselves already "close to $\mathbb{1}$". Indeed, let $g \mapsto T_g$ be a projective unitary representation of a continuous group. In other words:

$$T_{g_2}T_{g_1} = e^{i\lambda(g_1,g_2)}T_{g_2g_1}.$$

Evaluating this relation for

$$\frac{\mathrm{d}}{\mathrm{d}s}\Big|_s \frac{\mathrm{d}}{\mathrm{d}t}\Big|_t e^{sM_1}e^{tM_2}e^{-sM_1} = \frac{\mathrm{d}}{\mathrm{d}s}\Big|_{s=0}\Big(e^{sM_1}M_2e^{-sM_1}\Big) = [M_1,M_2].$$