

YET ANOTHER INTRODUCTION TO
QUANTUM FIELD THEORY
WITH THE EMPHASIS ON
THE REAL UNDERSTANDING OF VARIOUS NOTIONS
INCLUDING, BUT NOT RESTRICTED TO:
THE LOGIC OF THE SUBJECT
CANONICAL QUANTIZATION, PATH INTEGRALS
FEYNMAN DIAGRAMS
RENORMALIZATION AND REGULARIZATION
FROM TOY MODELS UP TO THE STANDARD MODEL
FOR THE USE OF STUDENTS
AND PARTICLE PHYSICISTS IN GENERAL
(BUT PERHAPS NOT THAT MUCH FOR PHILOSOPHERS S OR MATHEMATICIANS)

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ENJOY.

Preface

When I started giving lectures on quantum field theory, I had no intention of writing a book on the subject. There are plenty of such books already available on the market, and it seemed to make little sense to add another one. But, unfortunately, none of them was exactly to my taste (*The Quantum Theory of Fields* by Steven Weinberg did not suit that well as an introductory course and *Quantum Field Theory Lectures of Sidney Coleman* had not yet been printed). The standard modern textbook on the subject at that time was *An Introduction to Quantum Field Theory* by Peskin and Schroeder which, in my opinion, leaves too much to be desired.

So I started to write some notes to provide a set of hopefully useful comments and remarks to the lectures. Over the years, the notes were gradually expanded and supplemented, and eventually the text became more and more self-contained, until at some point it started to resemble a coherent set of lecture notes. The aim of the text is to explain not only what we are doing, but why we are doing it. I tried my best not to provide complicated answers to questions never asked. This applies not only to particular aspects of the subject, but also to the structure of the whole course.

In the rather extensive first part, almost no interesting particle physics is discussed at all. We only deal with scalar fields (spinless particles) and the emphasis is on the logic of the theory (with all the necessary technicalities, of course). In this part, students should learn and understand why and how we quantize classical fields, why and how the machinery of Feynman diagrams works, why and how we renormalize the parameters of Lagrangians, and why and how we utilize the path integral formulation of QFT.

The physics enters only in the second part, devoted to quantum electrodynamics. Here, the technical complications brought about by higher spins are discussed thoroughly, along with the important physical results. All this is done step by step. We start with spinless particles in a classical electromagnetic field, then the QED of spinless particles is developed, and only afterwards is the full (spinor) QED introduced.

The third part concerns the Standard Model. A large portion of this part, however, does not deal with the SM itself, but rather with particle physics before the SM. It is my firm belief that students exposed directly to the SM Lagrangian, with insufficient knowledge of the prior theoretical (and experimental) development, can miss the essence of the whole business. But it is not only the historical perspective that makes pre-SM particle physics so useful for an SM course. Virtually all the ingredients of the SM originated in pre-SM physics, and so they can be introduced in a quite natural way. Only once these ingredients are grasped to a reasonable level is the SM itself discussed.

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Part I

Basics of QFT (Spinless Particles)

Chapter 1

Introductions

Let us state at the very beginning that Quantum field theory is

- a theory of particles (in a way Quantum mechanics is a theory of atoms)¹
- mathematically ill-defined
- the most precise theory mankind ever had
- conceptually and technically quite demanding

Mainly because of the last feature, it seems reasonable to spend enough time with introductions. The reason for plural is that we shall try to introduce the subject in couple of different ways (in some sense independent, in some sense related to each another).

Our first introduction is in fact a summary. We shall try to show how QFT is used in practical calculations, without any attempt to understand why it is used in this way. The reason for this strange maneuver is that, surprisingly enough, it is much easier to grasp the bulk of QFT on this operational level than to really understand it. We believe that even a superficial knowledge of how QFT is usually used can be quite helpful in a subsequent, more serious, study of the subject. But it's probably worth saying that the first introduction can be skipped safely and returned to only after the Feynman rules were really derived in the subsequent chapters.

The second introduction is a brief exposition of the (mainly non-relativistic) many-particle quantum mechanics. This enables a natural introduction of many basic ingredients of QFT (the Fock space, creation and annihilation operators, calculation of vacuum expectation values, etc.) and simultaneously to avoid the difficult question of merging relativity and quantum theory.

It is the third introduction, which sketches that difficult question (merging relativity and quantum theory). Without going into technical details we try to describe how the notion of a relativistic quantum field enters the game in a kind of a natural way. The main goal of this third introduction is to clearly formulate the question, to which the canonical quantization provides an answer.

Only after these three introductions we shall try to develop QFT systematically. Initially, the development will concern only the scalar fields (spinless particles). More realistic theories for particles with spin $1/2$ and 1 are postponed to the subsequent parts of the book.

¹According to His Envyness, The High Inquisitor of Marseille, HSP (Hrdina Statočnej Práce) and SI unit of heterosexuality, may Peroon and other slavic gods bless Him forever — QFT is a theory of many other things, like e.g. an elephant ear, trunk, tail, etc.

In spite of the fact that His Envyness is sometimes quite a liar, here he is right. QFT can be defined in such a way (a useful one) that particles are not present from the beginning as basic building blocks, but they rather emerge (not neccessarily) as a feature of the theory. If so, the QFT is a theory of these particles.

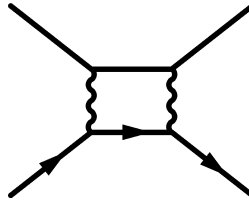
1.1 Conclusions

The machinery of QFT works like this:

- typical formulation of QFT — specification of a Lagrangian $\mathcal{L}$
- typical output of QFT — cross-sections $d\sigma/d\Omega$
- typical way of obtaining the output — Feynman diagrams

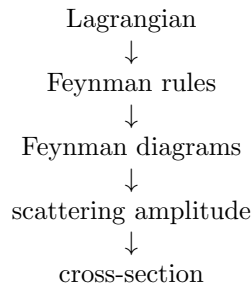
The machinery of Feynman diagrams works like this:

- For a given process (particle scattering, particle decay) there is a well defined set of pictures (graphs, diagrams). The set is infinite, but there is a simple criterion, allowing for identification of a relatively small number of the most important diagrams. Every diagram consists of several types of lines and several types of vertices. The lines either connect vertices (internal lines, propagators) or go out of the diagrams (external legs). An example:



- Every diagram has a number associated with it. The sum of these numbers is the so-called scattering amplitude. Once the amplitude is known, it is straightforward to obtain the cross-section — one just plugs the amplitude into a simple formula.
- The number associated with a diagram is the product of factors corresponding to the internal lines, external lines and the vertices of the diagram. Which factor corresponds to which element of the diagram is the content of the so-called Feynman rules. These rules are determined by the Lagrangian.

- The whole scheme is



- Derivation of the above scheme is a long and painful enterprise. Surprisingly enough, it is much easier to formulate the content of particular steps than to really derive them. And this formulation (without derivation²) is the theme of our introductory summary.

²It is perhaps worth mentioning that the direct formulation (without derivation) of the above scheme can be considered a fully sufficient formulation of the real content of QFT. This point of view is advocated in the famous Diagrammar by Nobel Prize winners 't Hooft and Veltman, where "*corresponding to any Lagrangian the rules are simply defined*"

1.1.1 Feynman rules

The role of the Lagrangian in QFT may be a sophisticated issue, but for the purposes of this summary the Lagrangian is just a set of letters containing the information about the Feynman rules. To decode this information one has to know, first of all, which letters represent fields (to know what the word *field* means is not necessary). For example, in the toy-model Lagrangian (of the so-called φ^3 -theory)

$$\mathcal{L}[\varphi] = \frac{1}{2}\partial_\mu\varphi\partial^\mu\varphi - \frac{1}{2}\mathring{m}^2\varphi^2 - \frac{1}{3!}\mathring{g}\varphi^3$$

the field is represented by the letter φ . Other symbols are whatever but not fields (as a matter of fact, they correspond to space-time derivatives, the so-called bare mass and the so-called bare coupling constant, but this is not important here). Another example is the Lagrangian of quantum electrodynamics (QED)

$$\mathcal{L}[\bar{\psi}, \psi, A_\mu] = \bar{\psi}(i\gamma^\mu\partial_\mu - \mathring{q}\gamma^\mu A_\mu - \mathring{m})\psi - \frac{1}{4}F_{\mu\nu}F^{\mu\nu} - \frac{1}{2\xi}(\partial_\mu A^\mu)^2$$

where $F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu$ and the fields are $\bar{\psi}$, ψ and A_μ (the symbol γ^μ stands for the so-called Dirac matrices, $\mathring{q}$ is the so-called bare charge and ξ is called a gauge parameter, but this information is not relevant here).

Now to the rules. Different fields are represented by different types of lines. The usual choice is a simple line for φ (called the scalar field), the wiggly line for A_μ (called in general the massless vector field, in QED the photon field) and a simple line with an arrow for $\bar{\psi}$ and ψ (called in general the spinor field, in QED usually the electron-positron field).

—————	φ
~~~~~	$A_\mu$
—————→	$\bar{\psi}, \psi$

The arrows are commonly used for complex fields, like  $\bar{\psi}$  and  $\psi$  (or  $\varphi^*$  and  $\varphi$ , if  $\varphi$  is complex)³. The arrow orientation is very important for external legs, where different orientations correspond to particles and antiparticles respectively (as we will see shortly). Every line is labelled by a momentum (and perhaps some other quantum numbers). The arrows discussed above and their orientation do not represent the momentum associated with the line!

The Feynman rules associate a specific factor with every internal line (propagator), line junction (vertex) and external line. Propagators are defined by the part of the Lagrangian quadratic in fields. Vertices are given by the rest of the Lagrangian. External line factor depends on the whole Lagrangian and usually (but not necessarily) it takes a form of the product of two terms. One of them is simple and is fully determined by the field itself, i.e. it does not depend on the details of the Lagrangian, while the other one is quite complicated and is determined by the whole Lagrangian.

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³Actually, in practice arrows are not used for scalar field, even if it is complex. The reason is that no factors depend on the arrows in this case, so people just like to omit them (although in principle the arrows should be present).

**vertices**

For a theory of one field  $\varphi$ , the factor corresponding to the  $n$ -leg vertex is⁴

$$n\text{-leg vertex} = i \left. \frac{\partial^n \mathcal{L}}{\partial \varphi^n} \right|_{\varphi \equiv 0}$$

For a theory with more fields, like QED, the definition is analogous, e.g. the vertex with  $l, m$  and  $n$  legs corresponding to  $\bar{\psi}, \psi$  and  $A_\mu$ -fields respectively, is

$$(l, m, n)\text{-legs vertex} = i \left. \frac{\partial^{l+m+n} \mathcal{L}}{\partial A_\mu^l \partial \psi^m \partial \bar{\psi}^n} \right|_{\text{fields} \equiv 0}$$

Each derivative with respect to a field produces a corresponding leg entering the vertex. For terms containing space-time derivative of a field, e.g.  $\partial_\mu \varphi$ , the derivative with respect to  $\varphi$  is defined in a bit bizarre way as⁵

$$\frac{\partial}{\partial \varphi} \partial_\mu \varphi \times \text{something} = -ip_\mu \times \text{something} + \partial_\mu \varphi \times \frac{\partial}{\partial \varphi} \text{something}$$

where  $p_\mu$  is the momentum (towards the vertex) of the leg produced by this derivative.

Clearly, examples are called for. In our toy-model given above (the so-called  $\varphi^3$ -theory) the non-quadratic part of the Lagrangian contains the third power of the field, so there will be only the 3-leg vertex

$$\begin{array}{c} \diagup \\ \bullet \\ \diagdown \end{array} \text{---} = i \frac{\partial^3}{\partial \varphi^3} \left( -\frac{1}{3!} \dot{g} \varphi^3 \right) = -i \dot{g}$$

In QED the non-quadratic part of the Lagrangian is  $-\bar{\psi} \hat{q} \gamma^\mu A_\mu \psi$ , leading to the single vertex

$$\begin{array}{c} \nearrow \\ \bullet \\ \nwarrow \end{array} \text{---} = i \frac{\partial^3 (-\bar{q} \bar{\psi} \gamma^\mu A_\mu \psi)}{\partial \bar{\psi} \partial \psi \partial A_\mu} = -i \hat{q} \gamma^\mu$$

and for purely didactic purposes, let us calculate the vertex for the theory with the non-quadratic Lagrangian given by  $-\dot{g} \varphi^2 \partial_\mu \varphi \partial^\mu \varphi$

$$\begin{aligned} \begin{array}{c} \diagup \\ \bullet \\ \diagdown \end{array} &= i \frac{\partial^4}{\partial \varphi^4} (-\dot{g} \varphi^2 \partial_\mu \varphi \partial^\mu \varphi) \\ &= -i \dot{g} \frac{\partial^3}{\partial \varphi^3} (2\varphi \partial_\mu \varphi \partial^\mu \varphi - 2i\varphi^2 p_1^\mu \partial_\mu \varphi) \\ &= -i \dot{g} \frac{\partial^2}{\partial \varphi^2} (2\partial_\mu \varphi \partial^\mu \varphi - 4i\varphi p_2^\mu \partial_\mu \varphi - 4i\varphi p_1^\mu \partial_\mu \varphi - 2\varphi^2 p_{1,\mu}^\mu) \\ &= -i 4\dot{g} \frac{\partial}{\partial \varphi} (-ip_3^\mu \partial_\mu \varphi - ip_2^\mu \partial_\mu \varphi - \varphi p_2 p_3 - ip_1^\mu \partial_\mu \varphi - \varphi p_1 p_3 - \varphi p_1 p_2) \\ &= 4i \dot{g} (p_1 p_2 + p_1 p_3 + p_1 p_4 + p_2 p_3 + p_2 p_4 + p_3 p_4) \end{aligned}$$

⁴The RHS of this definition could (should) contain a factor  $(2\pi)^4 \delta^4(p_1 + p_2 + \dots + p_n)$  where  $p_i$  is the momentum corresponding to the  $i$ -th leg (all momenta are understood to be pointing towards the vertex). However, we prefer to include this factor elsewhere.

⁵ $\frac{\partial}{\partial \varphi} \partial_\mu \varphi$  is by definition equal to  $-ip_\mu$ , and the Leibniz rule applies to  $\frac{\partial}{\partial \varphi}$ , as it should apply to anything worthy of the name derivative.

### propagators

Propagators are defined by the quadratic part of the Lagrangian. They are negative inverses of the 2-leg vertices with an  $i\varepsilon$  adornment (and with momenta  $p$  and  $p' = -p$  pointing towards the vertex)

$$\text{propagator} = i \left( \frac{\partial^2 \mathcal{L}}{\partial \varphi^2} \Big|_{\varphi=0, p'=-p} + i\varepsilon \right)^{-1}$$

The symbol  $\varepsilon$  stands for any positive infinitesimal quantity, therefore we will always replace  $\varepsilon \times \text{finite quantity}$  by the  $\varepsilon$  itself. For complex fields one uses  $\partial^2 \mathcal{L} / \partial \varphi^* \partial \varphi$ , definitions for other fields are similar.

The examples below are more than examples, they are universal tools to be used over and over. The point is that the quadratic parts of Lagrangians are the same in almost all theories, so once the propagators are calculated, they can be used in virtually all QFT calculations.

The quadratic part of the scalar field Lagrangian is given by  $\frac{1}{2} \partial_\mu \varphi \partial^\mu \varphi - \frac{1}{2} \dot{m}^2 \varphi^2$ , leading to  $\partial^2 \mathcal{L} / \partial \varphi^2|_{\varphi=0, p'=-p} = -p \cdot p' - \dot{m}^2|_{p'=-p} = p^2 - \dot{m}^2$ , i.e.

$$\text{---} = \frac{i}{p^2 - \dot{m}^2 + i\varepsilon}$$

The quadratic part of the spinor field Lagrangian is given by  $\bar{\psi} (i\gamma^\mu \partial_\mu - \dot{m}) \psi$ , leading to  $\partial^2 \mathcal{L} / \partial \bar{\psi} \partial \psi|_{\text{fields}=0, p'=-p} = \gamma^\mu p_\mu - \dot{m}$ , i.e.

$$\text{---} \rightarrow = \frac{i}{\gamma^\mu p_\mu - \dot{m} + i\varepsilon} = \frac{i(\gamma^\mu p_\mu + \dot{m})}{p^2 - \dot{m}^2 + i\varepsilon}$$

where we have utilized the identity  $(\gamma^\mu p_\mu - \dot{m})(\gamma^\mu p_\mu + \dot{m}) = p^2 - \dot{m}^2$ , which at this stage is just a God-given identity, allowing us to rewrite the propagator in the standard way with  $p^2 - \dot{m}^2 + i\varepsilon$  in the denominator.

Finally, for the massless vector field the quadratic Lagrangian is  $-\frac{1}{4} F_{\alpha\beta} F^{\alpha\beta} - \frac{1}{2\xi} (\partial_\alpha A^\alpha)^2$  leading to^{6,7,8}  $\partial^2 \mathcal{L} / \partial A_\mu \partial A_\nu|_{\text{fields}=0, p'=-p} = (1 - \frac{1}{\xi}) p^\mu p^\nu - p^2 \eta^{\mu\nu}$  where  $\eta^{\mu\nu}$  is the metric tensor

$$\text{~~~~~} = \frac{i}{\left(1 - \frac{1}{\xi}\right) p^\mu p^\nu - p^2 \eta^{\mu\nu} + i\varepsilon} = \frac{-i(\eta_{\mu\nu} - (1 - \xi) p_\mu p_\nu / p^2)}{p^2 + i\varepsilon}$$

Surprisingly enough, this is almost everything one would ever need as to the propagators. In the Standard Model, the spinor propagator describes quarks and leptons, the massless vector propagator describes photon and gluons, the scalar propagator describes the Higgs boson. The only missing propagator is the massive vector one, describing the  $W^\pm$  and  $Z^0$  bosons. This can be, however, worked out easily from the Lagrangian  $-\frac{1}{4} F_{\alpha\beta} F^{\alpha\beta} + \frac{1}{2} \dot{m}^2 A_\alpha A^\alpha$  (the result is  $-i(\eta^{\mu\nu} - p^\mu p^\nu / \dot{m}^2)(p^2 - \dot{m}^2 + i\varepsilon)^{-1}$ , the derivation is left as an exercise).

⁶For  $\mathcal{L} = \frac{1}{2} \left[ (\partial_\alpha A_\beta) (\partial^\beta A^\alpha) - (\partial_\alpha A_\beta) (\partial^\alpha A^\beta) - \frac{1}{\xi} (\partial_\alpha A^\alpha) (\partial_\beta A^\beta) \right]$  the derivatives are straightforward

$\frac{\partial \mathcal{L}}{\partial A_\mu} = -i \left( p_\alpha \eta_\beta^\mu \partial^\beta A^\alpha - p_\alpha \eta_\beta^\mu \partial^\alpha A^\beta - \frac{1}{\xi} p_\alpha \eta^{\alpha\mu} \partial_\beta A^\beta \right) = -i \left( p_\alpha \partial^\mu A^\alpha - p_\alpha \partial^\alpha A^\mu - \frac{1}{\xi} p^\mu \partial_\beta A^\beta \right)$

$\frac{\partial^2 \mathcal{L}}{\partial A_\mu \partial A_\nu} = -p_\alpha p'^\mu \eta^{\alpha\nu} + p_\alpha p'^\alpha \eta^{\mu\nu} + \frac{1}{\xi} p^\mu p'_\beta \eta^{\beta\nu} = p \cdot p' \eta^{\mu\nu} - p'^\mu p^\nu + \frac{1}{\xi} p^\mu p'^\nu$

⁷To find the matrix inverse to  $M^{\lambda\mu} = (1 - \xi^{-1}) p^\lambda p^\mu - p^2 \eta^{\lambda\mu}$  one may either make an educated guess  $M_{\mu\nu}^{-1} = A \eta_{\mu\nu} + B p_\mu p_\nu$  (there is nothing else at our disposal) and solve for  $A$  and  $B$ , or one may simply check that  $[(1 - \xi^{-1}) p^\lambda p^\mu - p^2 \eta^{\lambda\mu}] (-\eta_{\mu\nu} + (1 - \xi) p_\mu p_\nu / p^2) / p^2 = \eta_\nu^\lambda$ .

⁸Let us remark that without the term  $\frac{1}{2\xi} (\partial_\alpha A^\alpha)^2$  the propagator would not exist, since the 2-leg vertex would have no inverse. Two specific choices of the parameter  $\xi$  are known as the Feynman gauge ( $\xi = 1$ ) and the Landau gauge ( $\xi = 0$ ).

**external legs**

The factor corresponding to an external leg is, as a rule, the product of two factors. Let us start with the simpler one. For the scalar field  $\varphi$  (representing a particle with zero spin) this factor is the simplest possible, it equals to 1. For other fields (representing particles with higher spins) there is a nontrivial first factor for each external leg. This factor is different for particles and antiparticles. It also distinguishes between ingoing and outgoing particles (i.e. between the initial and the final state). The factor depends on the particle momentum and spin, but we are not going to discuss this dependence in any detail here.

As to the massless vector field  $A_\mu$  (e.g. for the photon, where antiparticle = particle) this factor is

ingoing particle	$\varepsilon_\mu$
outgoing particle	$\varepsilon_\mu^*$

For the spinor field (e.g. for the electron and positron, which are distinguished in diagrams by the orientation of the arrow) the factor is

ingoing particle	arrow towards the diagram	$u$
ingoing antiparticle	arrow out of the diagram	$\bar{v}$
outgoing particle	arrow out of the diagram	$\bar{u}$
outgoing antiparticle	arrow towards the diagram	$v$

These rules are universal, independent of the specific form of the Lagrangian.

Examples for electrons and photons may illuminate the general rules. We will draw diagrams from the left to the right, i.e. ingoing particles (initial state) are on the left and outgoing particles (final state) on the right⁹.

process	typical diagram	first external legs factors
$e^- \gamma \rightarrow e^- \gamma$		$u, \varepsilon_\mu, \bar{u}, \varepsilon_\nu^*$
$e^+ \gamma \rightarrow e^+ \gamma$		$\bar{v}, \varepsilon_\mu, v, \varepsilon_\nu^*$
$e^+ e^- \rightarrow e^+ e^-$		$\bar{v}, u, v, \bar{u}$
$e^- e^- \rightarrow e^- e^-$		$u, u, \bar{u}, \bar{u}$

⁹Note that some authors, including Peskin-Schroeder, draw the Feynman diagrams other way round, namely from the bottom to the top.

Now to the second factor corresponding to an external leg. It has a pretty simple appearance, namely it equals to  $\sqrt{Z}$ , where  $Z$  is a constant (the so-called wave-function renormalization constant) dependent on the field corresponding to the given leg. The definition and calculation of  $Z$  are, however, anything but simple.

Fortunately, the dominant part of vast majority of cross-sections and decay rates calculated by means of Feynman diagrams is given by the so-called tree diagrams (diagrams containing no closed loops), and at the tree level the  $Z$  constant is always equal to 1. So while staying at the tree level, one can forget about  $Z$  completely. And since our first aim is to master the tree level calculations, we can ignore the whole  $Z$ -affair until the discussion of loops and renormalization. The following sketch of the  $Z$  definition is presented only for the sake of completeness (and can be skipped safely at this moment).

Unlike all other Feynman rules, the  $Z$  constant is defined not directly via the Lagrangian, but rather via an infinite sum of Feynman diagrams¹⁰. The said sum, called the dressed propagator, contains all diagrams with two external legs corresponding to the field under consideration. These two external legs are treated in a specific way — the corresponding factor is not the external leg factor but rather the propagator. The dressed propagator is a function of the external leg momentum (both legs have the same momentum due to the vertex momentum  $\delta$ -functions) and, as a rule, has a pole in the  $p^2$ -variable. The residuum at this pole is the wanted  $Z$ .

This definition, as it stands, applies only to the scalar fields. For higher spins the dressed propagator is a matrix and the  $Z$  constant is defined via the eigenvalues of this matrix. So one can have, in principle, several different  $Z$  constants corresponding to one field. For the electron-positron field, however, there turns out to be only one such constant and the same is true for the photon field.

In addition to this, there is yet another very important ingredient in the external leg treatment. The external leg factor stands not only for the simple (bare) external leg, but rather for the dressed external leg (with all loop corrections). In other words, when calculating a scattering amplitude, one should not include diagrams with loop corrections on external legs. These diagrams are, in a sense, taken into account via the  $\sqrt{Z}$  factors¹¹.

Too complicated? Never mind. Simply forget everything about  $Z$ , it will be sufficient to recall it only much later, when dealing with renormalization.

**Remark:** *As we have indicated, in some circumstances the external leg factor may be even more complicated than the product of two terms (one of them being  $\sqrt{Z}$ ). This happens in presence of non-vanishing sums of all diagrams with two external legs corresponding to different fields. This is only rarely the case and always indicates that our choice of fields was not the most appropriate one. The remedy for this trouble is quite ordinary: after a suitable re-definition (just a simple linear combination) of the fields, the trouble simply drops out.*

---

¹⁰For the definition of Feynman diagrams see the next subsection.

¹¹After being forced to calculate the loop corrections to a simple line in order to obtain  $Z$ , one does not need to calculate them again when calculating the scattering amplitude. There is at least some justice in this world.

### 1.1.2 Feynman diagrams

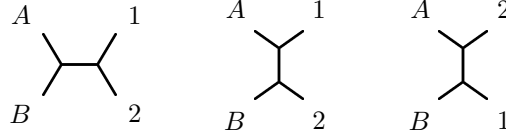
#### diagrams for a given process contributing at a given order

A process defines external legs, both ingoing and outgoing. A Feynman diagram corresponding to this process is any diagram (graph) with this set of external legs interconnected by the internal lines (propagators) of the theory, via the vertices of the theory, with exception of:

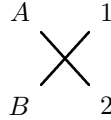
- diagrams with no vertices at all
- diagrams containing so-called "vacuum bubbles", i.e. subdiagrams not connected to any external leg
- diagrams containing so called "corrections on external legs", i.e. subdiagrams with two outgoing lines, one of which is an external leg

There is usually an infinite number of such diagrams. Still, only a finite number contribute at a given order. The order may be defined in at least three different ways, namely as **a)** the number of vertices, **b)** the power of the coupling constant or **c)** the number of (independent) loops. If there is only one type of vertex in the theory, these three definitions are equivalent¹². If one has more types of vertices, but all characterized by the same coupling constant¹³, then the first definition is not used and the other two are not equivalent.

As an example, let us consider a scattering  $AB \rightarrow 12$ , described by either  $\varphi^3$ - or  $\varphi^4$ -theory. At the leading order (the lowest nonzero order, tree level) one has for the  $\varphi^3$ -theory



while for the  $\varphi^4$ -theory ( $\mathcal{L}[\varphi] = \frac{1}{2}\partial_\mu\varphi\partial^\mu\varphi - \frac{1}{2}\hat{m}^2\varphi^2 - \frac{1}{4!}\hat{g}\varphi^4$ )

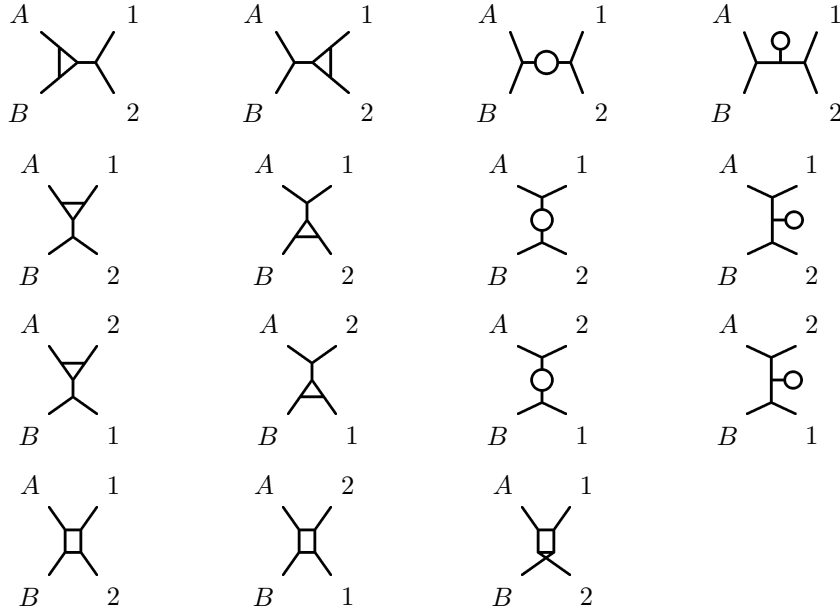


Note that the second and the third diagrams for the  $\varphi^3$ -theory are not equivalent, they contain different vertices (intersections of different lines).

¹²Proof: The equivalence of the first two definitions is evident (every vertex contributes by the same coupling constant). As to the equivalence of the third definition, let us denote the number of vertices, internal lines, external lines and independent loops by  $V$ ,  $I$ ,  $E$  and  $L$  respectively. The famous Euler's Theorem states  $V = I - L + 1$ . This is to be combined with  $nV = 2I + E$  where  $n$  is the number of legs of the vertex of the theory. The latter equation is nothing but a simple observation that we can count the number of lines by counting vertices and multiplying their number by  $n$ , but we are double-counting internal lines in this way. When combined, the equations give  $(n-2)V = 2L + E - 2$ , i.e. for a given  $E$  the dependence of  $V$  on  $L$  is linear.

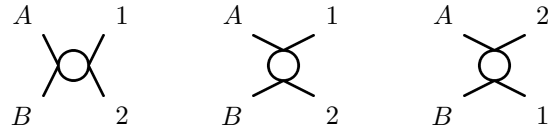
¹³A good example is the so-called scalar electrodynamics (spinless particles and photons) defined by the Lagrangian  $\mathcal{L}[\varphi] = (D_\mu\varphi)^* D^\mu\varphi - \hat{m}^2\varphi^*\varphi - \frac{1}{4}F_{\mu\nu}F^{\mu\nu} - \frac{1}{2\xi}(\partial_\mu A^\mu)^2$ , where  $D_\mu = \partial_\mu + i\hat{q}A_\mu$ .

At the next to leading order (1-loop level) one has for the  $\varphi^3$ -theory

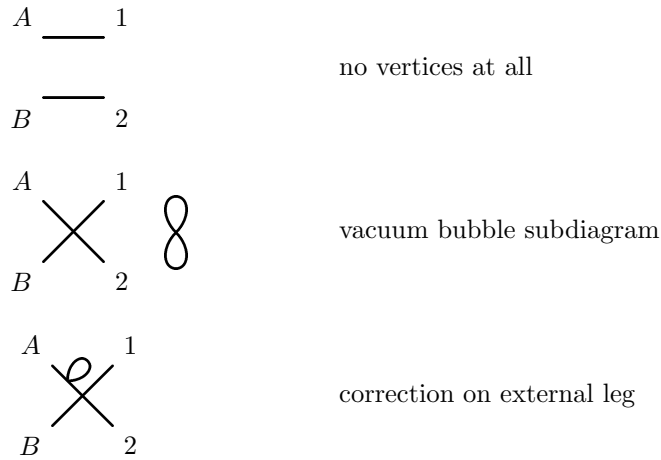


Note that in the last diagram the crossing of external legs  $B$  and  $2$  does not represent a vertex (we just did not manage to draw the diagram in plane without crossing). Let us remark that the 3 diagrams in the last column (so-called tadpole diagrams) are often omitted, since the factors corresponding to these diagrams usually turn out to vanish.

The next to leading order (1-loop level) result for the  $\varphi^4$ -theory is



As examples of diagrams not included among Feynman diagrams corresponding to the process under consideration let us mention



### the factor corresponding to a given diagram

The factor corresponding to a diagram is the product¹⁴ of factors corresponding to all external lines, internal lines and vertices of the diagram, multiplied by

- an extra factor  $(2\pi)^4 \delta^4(p_1 + p_2 + \dots + p_n)$  for each vertex ( $p_i$  is the momentum corresponding to the  $i$ -th leg, pointing towards the vertex).
- an extra factor  $\int \frac{d^4 k}{(2\pi)^4}$  for each propagator (with the four-momentum  $k$ )
- an extra so-called combinatorial factor, to be discussed later
- some extra factors of  $(-1)$  related to fermionic lines¹⁵

Examples¹⁶:

$$\begin{aligned}
 & \begin{array}{c} A \quad 1 \\ \diagdown \quad \diagup \\ B \quad 2 \end{array} = -i\hat{g}(2\pi)^4 \delta^4(p_A + p_B - p_1 - p_2) \\
 & \begin{array}{c} A \quad 1 \\ \diagdown \quad \diagup \\ B \quad 2 \end{array} = -\hat{g}^2 (2\pi)^8 \int \frac{d^4 k}{(2\pi)^4} \frac{i}{k^2 - \hat{m}^2 + i\varepsilon} \delta^4(p_A + p_B - k) \delta^4(k - p_1 - p_2) \\
 & \quad = -i \frac{\hat{g}^2}{(p_A + p_B)^2 - \hat{m}^2 + i\varepsilon} (2\pi)^4 \delta^4(p_A + p_B - p_1 - p_2) \\
 & \begin{array}{c} A \quad 1 \\ \diagdown \quad \diagup \\ B \quad 2 \end{array} = -\hat{g}^2 (2\pi)^8 \frac{1}{2} \int \frac{d^4 k}{(2\pi)^4} \frac{d^4 k'}{(2\pi)^4} \frac{i}{k^2 - \hat{m}^2 + i\varepsilon} \frac{i}{k'^2 - \hat{m}^2 + i\varepsilon} \delta^4(p_A + p_B - k - k') \times \\
 & \quad \quad \quad \uparrow \\
 & \quad \quad \quad \text{combinatorial factor} \quad \quad \quad \times \delta^4(k + k' - p_1 - p_2) \\
 & \quad = \frac{1}{2} \hat{g}^2 \int d^4 k \frac{1}{k^2 - \hat{m}^2 + i\varepsilon} \frac{1}{(p_A + p_B - k)^2 - \hat{m}^2 + i\varepsilon} \delta^4(p_A + p_B - p_1 - p_2) \\
 & \begin{array}{c} A \quad 1 \\ \diagdown \quad \diagup \\ B \quad 2 \end{array} = -\hat{q}^2 (2\pi)^8 \int \frac{d^4 k}{(2\pi)^4} \bar{u}_2 \gamma^\mu \delta^4(k - p_1 - p_2) \frac{i(\gamma^\lambda k_\lambda + \hat{m} + i\varepsilon)}{k^2 - \hat{m}^2 + i\varepsilon} \times \\
 & \quad \quad \quad \times \gamma^\nu \delta^4(p_A + p_B - k) u_B \varepsilon_{1,\mu}^* \varepsilon_{A,\nu} \\
 & \quad = -i\hat{q}^2 \frac{\bar{u}_2 \gamma^\mu (\gamma^\lambda (p_A + p_B)_\lambda + \hat{m}) \gamma^\nu u_B}{(p_A + p_B)^2 - \hat{m}^2 + i\varepsilon} \varepsilon_{1,\mu}^* \varepsilon_{A,\nu} (2\pi)^4 \delta^4(p_A + p_B - p_1 - p_2)
 \end{aligned}$$

¹⁴If individual factors are simple numbers, one does not care about their ordering. In some cases, however, these factors are matrices, and then the proper ordering is necessary. The basic rule here is that for every line with an arrow, the factors are to be ordered "against the arrow", i.e. starting from the end of the arrow and going in the reverse direction.

¹⁵The factor  $(-1)$  for every closed fermionic loop, and the relative minus sign for the diagrams, which can be obtained from each other by an interchange of two fermionic lines. Diagrams related to each other by the omission or addition of boson lines have the same sign.

¹⁶All momenta in these examples are understood to flow from the left to the right. One can, of course, choose another orientation of momenta and change the signs in  $\delta$ -functions correspondingly.

### the factor corresponding to a given diagram — an alternative formulation

There is another, a bit more economic way, of producing the factor corresponding to a given diagram. When using this method, diagrams are drawn in such a way that all the momentum  $\delta$ -functions in vertices are satisfied (e.g. in  $\varphi^3$ -theory instead of denoting legs going into the vertex as  $p_1, p_2, p_3$ , one denotes the third leg directly as  $-p_1 - p_2$ ). The factor corresponding to a diagram is the product of factors corresponding to all external lines, internal lines and vertices of the diagram, multiplied by

- an overall momentum  $\delta$ -function factor:  $(2\pi)^4 \delta(P_f - P_i)$   
( $P_i$  and  $P_f$  are sums of the ingoing and outgoing momenta respectively)
- an extra factor  $\int \frac{d^4 k}{(2\pi)^4}$  for each independent loop
- an extra so-called combinatorial factor, to be discussed later
- some extra factors of  $(-1)$  related to fermionic lines

The new rules are obtained from the previous ones by performing all trivial integrations over the vertex momentum  $\delta$ -functions. We will show now that after such integrations are performed one is indeed left with just the one non-integrated  $\delta$ -function and  $L$  (= number of independent loops) integrals yet to be evaluated.

Let us start with any internal line connecting two vertices. After integration over the momentum of this line, one gets rid of one of the vertex  $\delta$ -functions and the momentum of the line is fixed (in terms of the other momenta entering the vertex with the said  $\delta$ -function).

The reader may check, that in all the previous examples the results are obtained more directly with this formulation. The new rules are obtained from the previous one by performing all trivial integrations over the vertex  $\delta$ -functions. To see this, let us ignore all factors corresponding to a diagram except of momentum integrations for internal legs and momentum  $\delta$ -functions for vertices. Each integration corresponding to an internal line connecting two different vertices can now be depicted as omission of the corresponding internal line and merging two vertices into one vertex. Repeating this procedure over and over, one eventually gets rid of all internal lines connecting two different vertices. So finally one obtains a daisy-like diagram with only one vertex and some loopy internal lines going from this vertex and returning back. The number of these loops is the same, as the number of independent loops in the original diagram (this is due to the Euler's theorem  $L = I - V + 1$  and the fact that at each step the numbers  $I$  and  $V$  decrease by one). The remaining integrals are the loop-integrals mentioned in the alternative formulation. The  $\delta$ -function corresponding to the last vertex is the overall  $\delta$ -function. (Convince yourself about the last two statements.)

**combinatorial factors**

Beyond the tree level, a diagram may require the so-called combinatorial factor¹⁷, which is usually the most cumbersome factor to evaluate. Therefore, it seems reasonable to start with some simple rules of thumb:

- If two vertices are connected by  $n$  different internal lines, the corresponding combinatorial factor is  $1/n!$

$$\text{---} \bigcirc \text{---} \quad \frac{1}{3!} \qquad \text{---} \bigcirc \text{---} \quad \frac{1}{2!2!}$$

- If a line starts and ends in the same vertex, it contributes by  $1/2$  to the combinatorial factor

$$\text{---} \bigcirc \text{---} \quad \frac{1}{2} \qquad \text{---} \bigcirc \text{---} \quad \frac{1}{2} \frac{1}{2!}$$

- If  $N$  permutations of  $n$  internal vertices (i.e. vertices with no external legs) do not change the diagram, the corresponding combinatorial factor is  $1/N$  (note that if not all  $n!$  permutations leave the diagram untouched, then  $N \neq n!$ )

$$\text{---} \bigcirc \text{---} \quad \frac{1}{2} \frac{1}{3!} \qquad \text{---} \bigcirc \text{---} \quad \frac{1}{2^3} \frac{1}{3!}$$

- The above list is not exhaustive, e.g. it does not allow to find the correct combinatorial factor in the following case

$$\bigcirc \quad \frac{1}{8}$$

A systematic, but less illustrative, prescription goes something like this: Let us assign a label to each end of every line in the diagram. The labeled diagram is characterized by sets of labels belonging to the common vertex, and by pairs of labels connected by a line. Permutation of labels would typically lead to a diagram labeled in a different way. Some permutations, however, lead to the identically labeled diagram. Find out the number  $N$  of all such permutations (leaving the labeled diagram unchanged). The combinatorial factor of the diagram is  $1/N$ .

Needless to say, this prescription is not that easy to follow practically. Fortunately, in simple cases (and one seldom needs to go much further) it can be reduced easily to the above rules of thumb. To provide the reader with a systematic procedure of generating all diagrams with right combinatorial factors, we will formulate one such method in the next paragraph. If found too clumsy, the paragraph can be skipped safely.

¹⁷Why such a name: the diagrams represent specific terms of perturbative expansion, the number of terms corresponding to a given diagram is given by some combinatorics.

### an optional paragraph on drawing the diagrams with correct combinatorial factors

Let us consider diagrams with  $l$  external legs. We will represent the sum of all such diagrams (including diagrams with no vertices at all, diagrams containing vacuum bubbles and diagrams containing corrections on external legs) by a shaded blob with  $l$  legs.

Now let us focus on one of the external legs. What is it connected to? It can be connected either directly to one of the other external legs, or it goes to some  $m$ -leg vertex. In the former case, the sum of all diagrams equals to one leg with no vertices at all and the sum of all diagrams with  $l-2$  external legs (a simple line disconnected to a  $(l-2)$ -legged shaded blob). In the latter case, the sum of all diagrams contains this leg going to the said vertex and the sum of all diagrams with  $l+m-2$  external legs,  $m-1$  coming from the said vertex and  $l-1$  being true external legs (the vertex connected to a  $l+m-2$  shaded blob). If the external leg can go to different vertices, all of them has to be taken into account.

The combinatorial factors come as follows: If the vertex contains  $n_1, n_2, \dots$  non-external legs corresponding to the same field, then the combinatorial factor is  $1/(n_1! n_2! \dots)$ . The resulting relation is known as the Dyson-Schwinger equation. For the combined  $\varphi^3$ - and  $\varphi^4$ -theory it reads

$$\text{blob with } l \text{ legs} = \text{leg} + \dots + \text{blob with } l-2 \text{ legs} + \frac{1}{2!} \text{blob with } l \text{ legs} + \frac{1}{3!} \text{blob with } l \text{ legs}$$

To get all diagrams up to a given order with correct combinatorial factors, the DS equation is used in an iterative way: one starts the equation itself, then one takes any leg and applies the equation to it, then the same is repeated with some other leg etc., until one reaches

$$(\text{the structure one is interested in}) \times \text{blob} + \dots$$

with ellipsis standing for diagrams with disconnected external legs + higher orders.

Let us illustrate the procedure by the diagram with two external legs within the  $\varphi^4$ -theory. The starting point is the DS equation for 2 external legs

$$\text{blob with 2 legs} = \text{line} \times \text{blob} + \frac{1}{3!} \text{blob with 2 legs}$$

Now the DS equation is applied to some other leg, say to the 2nd external leg

$$\text{blob with 2 legs} = \text{line} \times \text{blob} + \frac{3}{3!} \text{blob with 2 legs} + \frac{1}{3!} \frac{1}{3!} \text{blob with 2 legs}$$

If we are interested only in the 1st order (in the number of vertices), then the last term is already of higher order, and the second term is again processed by the DS equation, to finally give

$$\text{blob with 2 legs} = \left( \text{line} + \frac{1}{2} \text{blob with 2 legs} \right) \times \text{blob} + \dots$$

The factor in front of the second diagram in the brackets is the correct combinatorial factor for this diagram. (As an exercise the reader may try to go one order higher.)

As another example let us consider the  $AB \rightarrow 12$  scattering within the  $\varphi^4$ -theory. Again, the starting point is the DS equation

$$\begin{array}{c} A \\ \diagup \quad \diagdown \\ \bullet \\ \diagdown \quad \diagup \\ B \end{array} \begin{array}{c} 1 \\ \\ \\ 2 \end{array} = \frac{1}{3!} \begin{array}{c} A \\ \diagup \quad \diagdown \\ \bullet \\ \diagdown \quad \diagup \\ B \end{array} \begin{array}{c} 1 \\ \\ \text{ellips} \\ 2 \end{array} + \dots$$

where the ellipsis stands for terms with disconnected external legs. The DS equation is now applied to some other leg, say the external leg  $B$

$$\begin{array}{c} A \\ \diagup \quad \diagdown \\ \bullet \\ \diagdown \quad \diagup \\ B \end{array} \begin{array}{c} 1 \\ \\ \\ 2 \end{array} = \frac{3}{3!} \begin{array}{c} A \\ \diagup \quad \diagdown \\ \bullet \\ \diagdown \quad \diagup \\ B \end{array} \begin{array}{c} 1 \\ \\ \text{ellips} \\ 2 \end{array} + \frac{1}{3!} \frac{1}{3!} \begin{array}{c} A \\ \diagup \quad \diagdown \\ \bullet \\ \diagdown \quad \diagup \\ B \end{array} \begin{array}{c} 1 \\ \\ \text{ellips} \\ 2 \end{array} + \dots$$

The RHS enjoys yet another DS equation, now say on the external leg 1, to give

$$\begin{array}{c} A \\ \diagup \quad \diagdown \\ \bullet \\ \diagdown \quad \diagup \\ B \end{array} \begin{array}{c} 1 \\ \\ \\ 2 \end{array} = \begin{array}{c} A \\ \diagup \quad \diagdown \\ \bullet \\ \diagdown \quad \diagup \\ B \end{array} \begin{array}{c} 1 \\ \\ \\ 2 \end{array} + \frac{1}{2} \frac{1}{3!} \begin{array}{c} A \\ \diagup \quad \diagdown \\ \bullet \\ \diagdown \quad \diagup \\ B \end{array} \begin{array}{c} 1 \\ \\ \text{ellips} \\ 2 \end{array} + \frac{1}{3!} \frac{3}{3!} \begin{array}{c} A \\ \diagup \quad \diagdown \\ \bullet \\ \diagdown \quad \diagup \\ B \end{array} \begin{array}{c} 1 \\ \\ \text{ellips} \\ 2 \end{array} + \frac{1}{3!} \frac{3}{3!} \begin{array}{c} A \\ \diagup \quad \diagdown \\ \bullet \\ \diagdown \quad \diagup \\ B \end{array} \begin{array}{c} 1 \\ \\ \text{ellips} \\ 2 \end{array} + \dots$$

The first two (last two) terms on the RHS come from the first (second) diagram on the RHS above, terms with more than two vertices are included into ellipsis. The first diagram is now treated with the help of the previous result for the 2-leg diagrams, the other three are treated all in the same way, which we will demonstrate only for the second diagram: we use the DS equation once more, now say for the external leg 2

$$\begin{aligned} \frac{1}{2} \frac{1}{2} \frac{1}{3!} \begin{array}{c} A \\ \diagup \quad \diagdown \\ \bullet \\ \diagdown \quad \diagup \\ B \end{array} \begin{array}{c} 1 \\ \\ \text{ellips} \\ 2 \end{array} &= \frac{2}{2} \frac{1}{2} \frac{1}{3!} \begin{array}{c} A \\ \diagup \quad \diagdown \\ \bullet \\ \diagdown \quad \diagup \\ B \end{array} \begin{array}{c} 1 \\ \\ \text{ellips} \\ 2 \end{array} + \frac{1}{2} \frac{3}{2} \frac{1}{3!} \begin{array}{c} A \\ \diagup \quad \diagdown \\ \bullet \\ \diagdown \quad \diagup \\ B \end{array} \begin{array}{c} 1 \\ \\ \text{ellips} \\ 2 \end{array} + \dots \\ &= \left( \frac{2}{2} \frac{3}{2} \frac{1}{2} \frac{1}{3!} \begin{array}{c} A \\ \diagup \quad \diagdown \\ \bullet \\ \diagdown \quad \diagup \\ B \end{array} \begin{array}{c} 1 \\ \\ \text{ellips} \\ 2 \end{array} + \frac{2}{2} \frac{3}{2} \frac{1}{2} \frac{1}{3!} \begin{array}{c} A \\ \diagup \quad \diagdown \\ \bullet \\ \diagdown \quad \diagup \\ B \end{array} \begin{array}{c} 1 \\ \\ \text{ellips} \\ 2 \end{array} \right) \times \begin{array}{c} \bullet \\ \diagdown \quad \diagup \\ \\ \end{array} + \dots \end{aligned}$$

Putting the pieces together, one finally obtains the one-loop diagrams with the correct combinatorial factors

$$\begin{array}{ccc} \frac{1}{2} \begin{array}{c} A \\ \diagup \quad \diagdown \\ \bullet \\ \diagdown \quad \diagup \\ B \end{array} \begin{array}{c} 1 \\ \\ \\ 2 \end{array} & \frac{1}{2} \begin{array}{c} A \\ \diagup \quad \diagdown \\ \bullet \\ \diagdown \quad \diagup \\ B \end{array} \begin{array}{c} 1 \\ \\ \\ 2 \end{array} & \frac{1}{2} \begin{array}{c} A \\ \diagup \quad \diagdown \\ \bullet \\ \diagdown \quad \diagup \\ B \end{array} \begin{array}{c} 1 \\ \\ \\ 2 \end{array} \\ \frac{1}{2} \begin{array}{c} A \\ \diagup \quad \diagdown \\ \bullet \\ \diagdown \quad \diagup \\ B \end{array} \begin{array}{c} 1 \\ \\ \text{ellips} \\ 2 \end{array} & \frac{1}{2} \begin{array}{c} A \\ \diagup \quad \diagdown \\ \bullet \\ \diagdown \quad \diagup \\ B \end{array} \begin{array}{c} 1 \\ \\ \text{ellips} \\ 2 \end{array} & \frac{1}{2} \begin{array}{c} A \\ \diagup \quad \diagdown \\ \bullet \\ \diagdown \quad \diagup \\ B \end{array} \begin{array}{c} 1 \\ \\ \text{ellips} \\ 2 \end{array} & \frac{1}{2} \begin{array}{c} A \\ \diagup \quad \diagdown \\ \bullet \\ \diagdown \quad \diagup \\ B \end{array} \begin{array}{c} 1 \\ \\ \text{ellips} \\ 2 \end{array} \end{array}$$

### 1.1.3 Scattering amplitude

The definition of the scattering amplitude  $M_{fi}$  is quite simple:

$$\text{the sum of Feynman diagrams} = iM_{fi} (2\pi)^4 \delta^{(4)}(P_f - P_i)$$

where  $P_i$  and  $P_f$  are the overall initial and final momentum respectively. By the sum of the diagrams, the sum of the corresponding factors is meant, of course.

Examples (to be checked by the reader):

•  $\varphi^3$ -theory,  $AB \rightarrow 12$  scattering

$$\text{tree-level } M_{fi} = -\frac{\dot{g}^2}{(p_A + p_B)^2 - \dot{m}^2 + i\varepsilon} - \frac{\dot{g}^2}{(p_A - p_1)^2 - \dot{m}^2 + i\varepsilon} - \frac{\dot{g}^2}{(p_A - p_2)^2 - \dot{m}^2 + i\varepsilon}$$

1-loop-level the result is intricate and not that illuminating  
but the reader is encouraged to work out some loop diagrams

•  $\varphi^4$ -theory,  $AB \rightarrow 12$  scattering

$$\text{tree-level } M_{fi} = -\dot{g}$$

$$\text{1-loop-level } M_{fi} = -\frac{1}{2}\dot{g}^2 [I(p_A + p_B) + I(p_A - p_1) + I(p_A - p_2)]$$

$$I(p) = i \int \frac{d^4 k}{(2\pi)^4} \frac{1}{k^2 - \dot{m}^2 + i\varepsilon} \frac{1}{(p-k)^2 - \dot{m}^2 + i\varepsilon}$$

•  $\varphi^2\Phi$ -theory¹⁸,  $A \rightarrow 12$  decay

$$\text{tree-level } A \text{ --- } \begin{array}{c} 1 \\ \diagdown \\ \diagup \\ 2 \end{array} \quad M_{fi} = -\dot{g}$$

$$\text{1-loop-level } A \text{ --- } \begin{array}{c} 1 \\ \diagdown \\ \diagup \\ 1 \\ \diagdown \\ \diagup \\ 2 \end{array} \quad M_{fi} = -\dot{g}^3 J(p_1, p_2)$$

$$J(p_1, p_2) = i \int \frac{d^4 k}{(2\pi)^4} \frac{1}{k^2 - \dot{M}^2 + i\varepsilon} \frac{1}{(p_1 + k)^2 - \dot{m}^2 + i\varepsilon} \frac{1}{(p_2 - k)^2 - \dot{m}^2 + i\varepsilon}$$

---

¹⁸A theory for two different fields  $\varphi$  and  $\Phi$ , defined by the Lagrangian

$$\mathcal{L}[\varphi, \Phi] = \frac{1}{2} \partial_\mu \varphi \partial^\mu \varphi - \frac{1}{2} \dot{m}^2 \varphi^2 + \frac{1}{2} \partial_\mu \Phi \partial^\mu \Phi - \frac{1}{2} \dot{M}^2 \Phi^2 - \frac{\dot{g}}{2} \varphi^2 \Phi$$

### 1.1.4 Cross-sections and decay rates

The cross-section for a scattering  $AB \rightarrow 12 \dots n$  is given by

$$d\sigma = (2\pi)^4 \delta^4(P_f - P_i) \frac{1}{4\sqrt{(p_A \cdot p_B)^2 - m_A^2 m_B^2}} |M_{fi}|^2 \prod_{i=1}^n \frac{d^3 p_i}{(2\pi)^3 2E_i}$$

while the analogous quantity for a decay  $A \rightarrow 12 \dots n$  is

$$d\Gamma = (2\pi)^4 \delta^4(P_f - P_i) \frac{1}{2E_A} |M_{fi}|^2 \prod_{i=1}^n \frac{d^3 p_i}{(2\pi)^3 2E_i}$$

where the so-called width  $\Gamma$  is related to the particle life-time  $\tau$  by  $\Gamma = 1/\tau$ .

Because of the  $\delta$ -function present in these formulae, one can relatively easily perform four integrations on the RHS. For the quite important case of  $n = 2$ , i.e. for  $AB \rightarrow 12$  and  $A \rightarrow 12$ , the result after such integrations is¹⁹ in the CMS (centre of mass system)

$$d\sigma_{\text{CMS}} = \frac{1}{64\pi^2} \frac{|\vec{p}_1|}{|\vec{p}_A|} \frac{1}{(p_A + p_B)^2} |M_{fi}|^2 d\Omega_1$$

$$d\Gamma_{\text{CMS}} = \frac{1}{32\pi^2} \frac{|\vec{p}_1|}{m_A^2} |M_{fi}|^2 d\Omega_1$$

while in the laboratory system (the rest frame of the target particle  $B$ )

$$d\sigma_{\text{lab}} = \frac{1}{64\pi^2} \frac{|\vec{p}_1|^2}{|\vec{p}_A|} \frac{1}{m_B} \frac{1}{(E_A + m_B) |\vec{p}_1| - E_1 |\vec{p}_A| \cos \vartheta} |M_{fi}|^2 d\Omega_1$$

and the formula for a decay is exactly the same as in the CMS (the two systems coincide in this case). All quantities (energies, momenta, angles) are, of course, understood in the corresponding frames and the non-present (integrated out)  $\delta$ -functions are understood to be satisfied.

**Remark:** *It is perhaps worth noticing that before  $\delta$ -function integrations the cross-section  $d\sigma$  is a product of Lorentz scalars (indeed  $\delta^4(P_f - P_i)$ ,  $(p_A \cdot p_B)^2 - m_A^2 m_B^2$ ,  $|M_{fi}|^2$  and  $d^3 p_i/2E_i$  are separately scalars), while  $d\Gamma$  is a product of scalars and one non-scalar quantity  $1/2E_A$ . After the integrations this neat structure is completely lost and this is the reason of the sad fact that one cannot simply and directly translate cross-sections and life-times from one frame to another.*

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¹⁹The specific formulae are obtained from the general ones by three trivial integrations over  $d^3 p_2$  leading to  $d\sigma = (2\pi)^4 \delta(E_1 + E_2 - E_A - E_B) \frac{1}{4\sqrt{(p_A \cdot p_B)^2 - m_A^2 m_B^2}} |M_{fi}|^2 \frac{d^3 p_1}{(2\pi)^3 2E_1} \frac{1}{(2\pi)^3 2E_2}$  with every  $\vec{p}_2$  replaced by  $-\vec{p}_1$  (in the CMS). Integration over the last  $\delta$ -function is usually performed in the spherical coordinates  $d^3 p_1 = k^2 dk d\Omega$  where  $k = |\vec{p}_1|$ . The last  $\delta$ -function is of the form  $\delta(g(k))$  with  $g(k) = \sqrt{k^2 + m_1^2} + \sqrt{k^2 + m_2^2} - E_A - E_B$ . This function is monotonous and it has therefore only one zero (iff  $m_1 + m_2 \leq E_A + E_B$ ), so one can write  $\delta(g(k)) = \delta(k - k_0)/|g'(k_0)|$  where  $g(k_0) = 0$ . Now  $g'(k) = k(E_1 + E_2)/E_1 E_2$  and after some algebra one gets in the CMS  $\sqrt{(p_A \cdot p_B)^2 - m_A^2 m_B^2} = |\vec{p}_A| (E_A + E_B)$ . All this together lead to the result for  $d\sigma_{\text{CMS}}$ , where  $|\vec{p}_1|$  is to be replaced everywhere (including  $M_{fi}$ ) by the zero point  $k_0$  of the  $g$ -function  $k_0 = \frac{1}{2} \sqrt{E_{\text{CMS}}^2 - 2(m_1^2 + m_2^2) + (m_1^2 - m_2^2)^2/E_{\text{CMS}}^2}$ . The result for  $d\Gamma_{\text{CMS}}$  is obtained in the same way. The calculation of the cross-section in the lab system is just slightly more cumbersome, due to  $\vec{p}_2 = \vec{p}_A - \vec{p}_1$ .

**Examples:**²⁰

- $\varphi^4$ -theory,  $AB \rightarrow 12$  scattering, tree level

$$d\sigma_{\text{CMS}} = \frac{1}{64\pi^2} \frac{1}{s} g^2 d\Omega \quad s = (p_A + p_B)^2$$

In this case the differential cross-section does not depend on angles, so one can immediately write down the total cross-section  $\sigma_{\text{CMS}} = g^2/16\pi s$ .

- $\varphi^3$ -theory,  $AB \rightarrow 12$  scattering, tree level

$$d\sigma_{\text{CMS}} = \frac{g^4}{64\pi^2 s} \left( \frac{1}{s-m^2} + \frac{1}{t-m^2} + \frac{1}{u-m^2} \right)^2 d\Omega \quad \begin{aligned} t &= (p_A - p_1)^2 \\ u &= (p_A - p_2)^2 \end{aligned}$$

where  $s, t, u$  are the frequently used so-called Mandelstam variables.

**Exercises:**

- $AB \rightarrow 12$  scattering at the tree level, within "the  $\varphi^4$ -theory with derivatives", i.e. the theory of scalar fields with the non-quadratic part of the Lagrangian  $\mathcal{L}_{\text{int}} = -\frac{g}{4}\varphi^2\partial_\mu\varphi\partial^\mu\varphi$ .
- $\Phi \rightarrow \varphi\varphi$  decay rate,  $\varphi\varphi \rightarrow \varphi\varphi$ ,  $\varphi\Phi \rightarrow \varphi\Phi$  and  $\varphi\varphi \rightarrow \Phi\Phi$  cross-sections at the tree level, for the  $\varphi^2\Phi$ -theory defined in the footnote on the page 17.

At this point we have achieved the goal of the first introduction – we are able to perform some basic calculations for particle scattering and/or decays, even if only at the level of following a cookbook-recipe. In the second introduction, which comes right after, we will learn what physics does the recipe come from – it will turn out be just a specific kind of a perturbation theory in multi-particle quantum theories.

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²⁰In final results the limit  $\varepsilon \rightarrow 0$  is usually understood, therefore there are no  $i\varepsilon$  terms in propagators.

## 1.2 Many-Body Quantum Mechanics

The main characters of QFT are quantum fields or perhaps creation and annihilation operators (since the quantum fields are some specific linear combinations of the creation and annihilation operators). In most of the available textbooks on QFT, the creation and annihilation operators are introduced in the process of the so-called canonical quantization²¹. This, however, is not the most natural way. In opinion of the present author, it may be even bewildering, as it may distort the student's picture of relative importance of basic ingredients of QFT (e.g. by overemphasizing the role of the canonical quantization). The aim of this second introduction is to present a more natural definition of the creation and annihilation operators, and to demonstrate their main virtues.

### 1.2.1 Fock space, creation and annihilation operators

#### Fock space

##### 1-particle system

the states constitute a Hilbert space  $\mathcal{H}^1$  with an orthonormal basis  $|i\rangle$ ,  $i \in N$

##### 2-particle system²²

the states constitute the Hilbert space  $\mathcal{H}^2$  or  $\mathcal{H}_B^2$  or  $\mathcal{H}_F^2$ , with the basis  $|i, j\rangle$

non-identical particles	$\mathcal{H}^2 = \mathcal{H}^1 \otimes \mathcal{H}^1$	$ i, j\rangle =  i\rangle \otimes  j\rangle$
identical bosons	$\mathcal{H}_B^2 \subset \mathcal{H}^1 \otimes \mathcal{H}^1$	$ i, j\rangle = \frac{1}{\sqrt{2}}( i\rangle \otimes  j\rangle +  j\rangle \otimes  i\rangle)$
identical fermions	$\mathcal{H}_F^2 \subset \mathcal{H}^1 \otimes \mathcal{H}^1$	$ i, j\rangle = \frac{1}{\sqrt{2}}( i\rangle \otimes  j\rangle -  j\rangle \otimes  i\rangle)$

##### $n$ -particle system (identical particles)

the Hilbert space is either  $\mathcal{H}_B^n$  or  $\mathcal{H}_F^n \subset \underbrace{\mathcal{H}^1 \otimes \dots \otimes \mathcal{H}^1}_n$ , with the basis

$$|i, j, \dots, k\rangle = \frac{1}{\sqrt{n!}} \sum_{\text{permutations}} (\pm 1)^p \underbrace{|i\rangle \otimes |j\rangle \otimes \dots \otimes |k\rangle}_n$$

where  $p$  is the parity of the permutation, the  $\begin{smallmatrix} \text{upper} \\ \text{lower} \end{smallmatrix}$  sign applies to  $\begin{smallmatrix} \text{bosons} \\ \text{fermions} \end{smallmatrix}$

##### 0-particle system

1-dimensional Hilbert space  $\mathcal{H}^0$  with the basis vector  $|0\rangle$  (no particles, vacuum)

##### Fock space

direct sum of the bosonic or fermionic  $n$ -particle spaces

$$\mathcal{H}_B = \bigoplus_{n=0}^{\infty} \mathcal{H}_B^n \qquad \mathcal{H}_F = \bigoplus_{n=0}^{\infty} \mathcal{H}_F^n$$

²¹There are exceptions. In the Weinberg's book the creation and annihilation operators are introduced exactly in the spirit we are going to adopt in this section. The same philosophy is to be found in some books on many-particle quantum mechanics. On the other hand, some QFT textbooks avoid the creation and annihilation operators completely, sticking exclusively to the path integral formalism.

²²This is the keystone of the whole structure. Once it is really understood, the rest follows smoothly. To achieve a solid grasp of the point, the reader may wish to consult the couple of remarks following the definition of the Fock space.

**Remark:** Let us recall that for two linear spaces  $U$  (basis  $e_i$ , dimension  $m$ ) and  $V$  (basis  $f_j$ , dimension  $n$ ), the direct sum and product are linear spaces  $U \oplus V$  (basis generated by both  $e_i$  and  $f_j$ , dimension  $m + n$ ) and  $U \otimes V$  (basis generated by ordered pairs  $(e_i, f_j)$ , dimension  $m.n$ ).

**Remark:** The fact that the Hilbert space of a system of two non-identical particles is the direct product of the 1-particle Hilbert spaces may come as not completely obvious. If so, it is perhaps a good idea to start from the question what exactly the 2-particle system is (provided that we know already what the 1-particle system is). The answer within the quantum physics is not that straightforward as in the classical physics, simply because we cannot count the quantum particles directly, e.g. by pointing the index finger and saying one, two. Still, the answer is not too complicated even in the quantum physics. It is natural to think of a quantum system as being 2-particle iff

a) it contains states with sharp quantum numbers (i.e. eigenvalues of a complete system of mutually commuting operators) of both 1-particle systems, and this holds for all combinations of values of these quantum numbers

b) such states constitute a complete set of states

This, if considered carefully, is just the definition of the direct product.

**Remark:** A triviality which, if not explicitly recognized, can mix up one's mind:  $\mathcal{H}^1 \cap \mathcal{H}^2 = \emptyset$ , i.e. the 2-particle Hilbert space contains no vectors corresponding to states with just one particle, and vice versa.

**Remark:** The fact that multiparticle states of identical particles are represented by either completely symmetric or completely antisymmetric vectors should be familiar from the basic QM course. The former case is called bosonic, the latter fermionic. In all formulae we will try, in accord with the common habit, to treat these two possibilities simultaneously, using symbols like  $\pm$  and  $\mp$ , where the upper and lower signs apply to bosons and fermions respectively.

**Remark:** As to the basis vectors, our notation is not the only possible one. Another widely used convention (the so-called occupation number representation) denotes the basis vectors as  $|n_1, n_2, \dots\rangle$ , where  $n_i$  is the number of particles in the  $i$ -th 1-particle state. So e.g.  $|2, 2, 2, 4, 4\rangle \Leftrightarrow |0, 3, 0, 2, 0, 0, 0, \dots\rangle$ , where the LHS is in our original notation while the RHS is in the occupation number representation. The main drawback of the original notation is that it is not unique, e.g.  $|1, 2, 3\rangle$  and  $\pm|1, 3, 2\rangle$  denotes the same vector. One should be therefore careful when summing over all basis states. The main drawback of the occupation number representation is typographical: one cannot write any basis vector without the use of ellipsis, and even this may sometimes become unbearable (try e.g. to write  $|49, 87, 642\rangle$  in the occupation number representation).

**Remark:** The basis vectors  $|i, j, \dots, k\rangle$  or  $|n_1, n_2, \dots\rangle$  are not all normalized to unity (they are, but only if all  $i, j, \dots, k$  are mutually different, i.e. if none of  $n_i$  exceeds 1). If some of the  $i, j, \dots, k$  are equal, i.e. if at least one  $n_i > 1$ , then the norm of the fermionic state is automatically zero (this is the Pauli exclusion principle), while the norm of the bosonic state is  $\sqrt{n_1! n_2! \dots}$ . Prove this.

**Remark:** A triviality which, if not explicitly recognized, can mix up one's mind: the vacuum  $|0\rangle$  is a unit vector which has nothing to do with the zero vector 0.

### creation and annihilation operators

Let  $|i\rangle$  ( $i = 1, 2, \dots$ ) be an orthonormal basis of a 1-particle Hilbert space, and  $|0\rangle, |i\rangle, |i, j\rangle, |i, j, k\rangle, \dots$  ( $i \leq j \leq k \leq \dots$ ) an orthogonal basis of the Fock space. The creation and annihilation operators are defined as follows

creation operator  $a_i^+$

is a linear operator, which maps the  $n$ -particle basis vector to the  $(n + 1)$ -particle vector by adding one particle in the  $i$ -th state (the particle is added at the first position in the resulting vector; for bosons this rule does not matter, for fermions it determines the sign)

$$a_i^+ |0\rangle = |i\rangle \quad a_i^+ |j\rangle = |i, j\rangle \quad a_i^+ |j, k, \dots\rangle = |i, j, k, \dots\rangle$$

annihilation operator  $a_i$

is a linear operator, which maps the  $n$ -particle basis vector to the  $(n - 1)$ -particle vector by removing one particle in the  $i$ -th state. The particle is removed from the first position of the original vector, and if it is not there, the original vector must be reshuffled (for bosons this rule does not matter, for fermions it determines the sign). If the original vector contains more than one particle in the  $i$ -th state, the whole procedure is performed with each of them and the results are summed up. If the original vector does not contain a particle in the  $i$ -th state, the result is the zero vector.

$$\begin{aligned} a_i |0\rangle &= 0 & a_i |j\rangle &= \delta_{ij} |0\rangle \\ a_i |j, k, l, \dots\rangle &= \delta_{ij} |k, l, \dots\rangle \pm \delta_{ik} |j, l, \dots\rangle + \delta_{il} |j, k, \dots\rangle \pm \dots \end{aligned}$$

Both creation and annihilation operators are linear and they are defined on the basis vectors. Consequently they are defined for any vector.

**Remark:** In the occupation number representation, the definitions read

$$\begin{aligned} \text{bosons} \quad a_i^+ |n_1, \dots, n_i, \dots\rangle &= |n_1, \dots, n_i + 1, \dots\rangle \\ a_i |n_1, \dots, n_i, \dots\rangle &= n_i |n_1, \dots, n_i - 1, \dots\rangle \\ \text{fermions} \quad a_i^+ |n_1, \dots, n_i = 0, \dots\rangle &= (-1)^{p_i} |n_1, \dots, n_i = 1, \dots\rangle \\ a_i^+ |n_1, \dots, n_i = 1, \dots\rangle &= 0 \\ a_i |n_1, \dots, n_i = 0, \dots\rangle &= 0 \\ a_i |n_1, \dots, n_i = 1, \dots\rangle &= (-1)^{p_i} |n_1, \dots, n_i = 0, \dots\rangle \\ p_i &= \sum_{k=1}^{i-1} n_k \end{aligned}$$

Creation and annihilation operators are very useful, because

- they enable the most natural description of processes in which the number of particles is not conserved, i.e. in which particles are created and/or destroyed
- any linear operator can be expressed in terms of the creation and annihilation operators, namely as a sum of products of these operators
- there is a standard and routine method of how to calculate matrix elements of operators expressed in terms of the creation and annihilation operators.

In view of how frequent the processes of particle creation and annihilation are (decays and inelastic scatterings in the atomic, nuclear, subnuclear and solid state physics), the first point is evidently very important. And in view of how often the QM calculations are just the calculations of various matrix elements of linear operators, the other two points are clearly also very important.

**key attributes of the creation and annihilation operators**

Perhaps the three most important are²³

- $a_i^+ = a_i^\dagger$  i.e.  $a_i^+$  and  $a_i$  are Hermitian conjugated
- $a_i^+ a_i$  (no summation) is the operator of number of particles in the  $i$ -th state (and consequently  $\sum_i a_i^+ a_i$  is the operator of the overall number of particles)
- $[a_i, a_j^+]_{\mp} = \delta_{ij}$        $[a_i, a_j]_{\mp} = [a_i^+, a_j^+]_{\mp} = 0$       where  $[x, y]_{\mp} = xy \mp yx$

The proof is an easy and very useful exercise, recommended to anybody who wants to become quickly accustomed to elementary manipulations with the  $a_i^+, a_i$  operators. The following sketch of the proof is therefore intended only as a check of reader's own work (the proof is performed in the occupation number formalism, which is more convenient for this purpose).

- Hermitian conjugation

$$\begin{aligned} \langle \dots n'_i \dots | a_i | \dots n_i \dots \rangle &= \langle \dots n'_i \dots | n_i - 1 \dots \rangle n_i = \langle \dots | \dots \rangle (n_i - 1)! n_i \delta_{n'_i, n_i - 1} \\ \langle \dots n_i \dots | a_i^+ | \dots n'_i \dots \rangle &= \langle \dots n_i \dots | n'_i + 1 \dots \rangle = \langle \dots | \dots \rangle n_i! \delta_{n_i, n'_i + 1} \end{aligned}$$

where for bosons  $n_i, n'_i \in N$  and for fermions  $n_i, n'_i \in \{0, 1\}$

- particle number operator

bosons

$$a_i^+ a_i | \dots n_i \dots \rangle = a_i^+ n_i | \dots n_i - 1 \dots \rangle = n_i a_i^+ | \dots n_i - 1 \dots \rangle = n_i | \dots n_i \dots \rangle$$

fermions

$$a_i^+ a_i | \dots 0 \dots \rangle = 0$$

$$a_i^+ a_i | \dots 1 \dots \rangle = a_i^+ (-1)^{p_i} | \dots 0 \dots \rangle = (-1)^{2p_i} | \dots 1 \dots \rangle$$

- (anti)commutation relation

bosons

$$\begin{aligned} [a_i, a_i^+] | \dots n_i \dots \rangle &= a_i | \dots n_i + 1 \dots \rangle - n_i a_i^+ | \dots n_i - 1 \dots \rangle \\ &= (n_i + 1) | \dots n_i \dots \rangle - n_i | \dots n_i \dots \rangle = | \dots n_i \dots \rangle \\ [a_i, a_j^+] | \dots n_i \dots n_j \dots \rangle &= a_i | \dots n_i \dots n_j + 1 \dots \rangle - a_j^+ n_i | \dots n_i - 1 \dots n_j \dots \rangle \\ &= n_i | \dots n_i - 1 \dots n_j + 1 \dots \rangle - n_i | \dots n_i - 1 \dots n_j + 1 \dots \rangle = 0 \end{aligned}$$

fermions

$$\begin{aligned} \{a_i, a_i^+\} | \dots 1 \dots \rangle &= 0 + (-1)^{p_i} a_i^+ | \dots 0 \dots \rangle = (-1)^{2p_i} | \dots 1 \dots \rangle = | \dots 1 \dots \rangle \\ \{a_i, a_i^+\} | \dots 0 \dots \rangle &= (-1)^{p_i} a_i | \dots 1 \dots \rangle + 0 = (-1)^{2p_i} | \dots 0 \dots \rangle = | \dots 0 \dots \rangle \\ \{a_i, a_j^+\} | \dots 0 \dots 0 \dots \rangle &= (-1)^{p_j} a_i | \dots 0 \dots 1 \dots \rangle + 0 = 0 \\ \{a_i, a_j^+\} | \dots 0 \dots 1 \dots \rangle &= 0 \\ \{a_i, a_j^+\} | \dots 1 \dots 0 \dots \rangle &= (-1)^{p_i + p_j} | \dots 0 \dots 1 \dots \rangle + (-1)^{p_i + p_j - 1} | \dots 0 \dots 1 \dots \rangle = 0 \\ \{a_i, a_j^+\} | \dots 1 \dots 1 \dots \rangle &= 0 + (-1)^{p_i} a_j^+ | \dots 0 \dots 1 \dots \rangle = 0 \end{aligned}$$

The other (anti)commutation relations are treated in the same way.

²³Note that  $a_i^+$  and  $a_i$  operators could be (and often are) introduced in the reversed order. In that case, the (anti)commutation relations are postulated and the Fock space is constructed afterwards for  $a_i^+$  and  $a_i$  to have something to live in. It is perhaps just a matter of taste, but the present author strongly prefers the "more natural logic" of this section. Later in these lectures, however, we will encounter also the reversed logic of the canonical quantization.

### creation and annihilation vs. raising and lowering operators

The reader is perhaps already familiar with operators  $a^+$  and  $a$  satisfying the above commutation relations. Such operators are introduced for the LHO (linear harmonic oscillator) in every basic QM course²⁴. What is the relation between the LHO raising and lowering operators (commonly known also as ladder operators) and our creation and annihilation operators? Three important points are to be emphasized:

1. The creation and annihilation operators have (in principle) nothing to do with the LHO ladder operators. They are naturally defined (as we have seen) in the Fock space without any reference to (or even presence of) harmonic oscillators.
2. The definition of raising and lowering operators (with the  $m\omega$  factor replaced by an arbitrary real number  $\lambda$ ) applies to any 1-particle system, not only to the LHO. Indeed, for  $a^+$  and  $a$  defined as

$$a^+ = \sqrt{\frac{\lambda}{2\hbar}} \hat{x} - \frac{i}{\sqrt{2\hbar\lambda}} \hat{p} \qquad a = \sqrt{\frac{\lambda}{2\hbar}} \hat{x} + \frac{i}{\sqrt{2\hbar\lambda}} \hat{p}$$

one can show (just like in the case of LHO) that

- (a) they are hermitian conjugate to each other
- (b) the canonical commutation relation  $[\hat{x}, \hat{p}] = i\hbar$  implies  $[a, a^+] = 1$
- (c) the eigenvalues of the operator  $\hat{N} = a^+a$  are natural numbers plus zero

Let us stress that the definition of these operators have nothing to do with the LHO. What makes the LHO special in this respect is the Hamiltonian, which is exceptionally simple in terms of  $a^+$ ,  $a$ . But ladder operators can be useful for any system. Naturally, they are most useful for systems "close to the LHO", where the difference in Hamiltonians can be treated as a small perturbation.

3. In spite of the first two points the creation and annihilation operators are usually closely related to the ladder operators. The reason is twofold.
  - (a) The LHO ladder operators can be viewed as the creation and annihilation operators of some formal particles in some bizarre states. The point is that LHO is formally equivalent to the ideal gas of arbitrary number of formal particles, all of which can be, however, in just one state. This is a simple consequence of equidistant spectrum of the LHO Hamiltonian (the  $n$ -th excited state of the LHO can be treated as a state of  $n$  formal particles with equal energies)
  - (b) Any ideal gas is in some sense equivalent to a system of harmonic oscillators. The point is that when expressed in terms of creation and annihilation operators, the Hamiltonian of an ideal gas is equivalent to the Hamiltonian of several formal harmonic oscillators. This will follow from the explicit form of the ideal gas Hamiltonian which we shall derive in the next section.

Due to the point 3b the LHO ladder operators play an important (even if only an auxiliary) role in one particular development of QFT, namely in the canonical quantization of classical fields (we will learn a lot about it later on). Since this is perhaps the most common development of the theory, the role of the LHO ladder operators can be easily overestimated. Let us therefore stress once more that creation and annihilation operators do not need any mention of LHO whatsoever.

²⁴Recall  $a^+ = \hat{x}\sqrt{m\omega/2\hbar} - i\hat{p}/\sqrt{2\hbar m\omega}$ ,  $a = \hat{x}\sqrt{m\omega/2\hbar} + i\hat{p}/\sqrt{2\hbar m\omega}$  and they are by definition conjugated to each other. The canonical commutation relation  $[\hat{x}, \hat{p}] = i\hbar$  implies for  $a^+$  and  $a$  the commutation relation of the creation and annihilation operators and the eigenvalues of the operator  $N = a^+a$  are natural numbers plus zero (this follows from the commutation relation).

**Remark:** It may come as a kind of miracle that the specific complex linear combinations of  $x(t)$  and  $p(t)$  solve the spectrum of the LHO Hamiltonian so efficiently (as everybody knows from an elementary QM course). In quantum mechanics these linear combinations come out of thin air and they are, frankly speaking, quite mysterious. But at the classical level they are not as artificial as they may appear at the first sight. It is quite common to write down the solution of the classical equation of motion for LHO in the complex form as  $x(t) = Ae^{-i\omega t} + Be^{i\omega t}$  and  $p(t) = -im\omega(Ae^{-i\omega t} - Be^{i\omega t})$  (both  $x(t)$  and  $p(t)$  are in general complex, but if one starts with real initial conditions, then  $B = A^*$ , and they remain real forever). Now one sees that linear combinations  $x(t) + \frac{i}{m\omega}p(t) = 2Ae^{-i\omega t}$  and  $x(t) - \frac{i}{m\omega}p(t) = 2Be^{i\omega t}$  are just two independent classical solutions. It is therefore not so much surprising that the linear combinations inspired by the classical solutions (even if rescaled by the factor  $\sqrt{m\omega/2\hbar}$ )²⁵ solve the problem relatively quickly also at the quantum level.

**Remark:** The previous remark did not investigate any deep connection between the classical and quantum physics, it was just a rough classical inspiration of the notoriously known treatment of the quantum LHO. We will have more to say about formal connections between the classical and quantum physics,²⁶ but it is worth emphasizing that at this point our discussion is purely quantum. The same applies to the following remark on phonons, which is again purely quantum (in spite of the fact that many authors start the discussion of phonons at the classical level).

**Remark:** An ideal gas of formal particles, which arises more or less naturally in discussion of LHO, is even more appealing in case of coupled harmonic oscillators. And this is indeed a very important case, due to the famous miracle of systems in the vicinity of their stable equilibria: any such system is well approximated by the system of coupled harmonic oscillators which, in turn, is equivalent to the system of decoupled harmonic oscillators.

Stationary states of the system of the independent harmonic oscillators are characterized by the sequence  $(N_1, N_2, \dots)$  where  $N_n$  defines the energy level of the  $n$ -th oscillator. Energies of individual oscillators are  $\hbar\omega_n(N_n + 1/2)$ . Energy of the system is  $\sum_n \hbar\omega_n(N_n + 1/2)$ .

Now let us imagine a system of free particles, each of them having energy eigenstates labeled by  $n$  with eigenvalues  $\hbar\omega_n$ . If there are  $N_n$  particles in the  $n$ -th state, the energy of the system will be  $\sum_n \hbar\omega_n N_n$ . This is equivalent (up to a constant) to the Hamiltonian of independent oscillators. It is common habit to describe a system of independent harmonic oscillators in terms of the equivalent system of free formal particles. These formal particles are called phonons.

Phonons are would-be particles (often called quasiparticles or collective excitations) widely used for the formal description of real particles behaving as coupled harmonic oscillators (e.g. nuclei or positive ions in a crystal lattice). These formal particles may look like real ones, especially in systems with translational symmetry. In such systems decoupling of oscillators is provided by the Fourier transformation, which brings (quasi)momentum in the game.²⁷ In that case phonons behave like having well defined energy and (quasi)momentum. Nevertheless, phonon is not a kind of particle. Strictly speaking, it is just a word.

²⁵In this section we are going to use explicit  $\hbar$ , just to make comparison with standard QM textbooks easier.

²⁶At the end of this section we will discuss an important issue of the classical limit of a quantum theory. The whole second chapter will be, on the other hand, devoted to the reverse procedure, namely to the canonical technique of obtaining a quantum theory from a given classical one. But to appreciate the logic of this Introduction, it is important to be aware of the fact that no classical physics as a starting point is involved.

²⁷Many remarks in this second introduction presume a reader with a basic knowledge of the solid state theory. For those readers who are not familiar with the quoted notions, the Appendix ?? is intended to fill the gap at least to some minimal extent.

### creation and annihilation operators in different bases

So far our definition of the creation and annihilation operators was based on the specific choice of basis in the 1-particle Hilbert space  $\mathcal{H}^1$ . Have we started from some other orthonormal basis, we would get a different set of creation and annihilation operators. What is the relation between the two sets of these operators?

Let  $|\alpha\rangle$  ( $\alpha \in N$ ) be an orthonormal basis of  $\mathcal{H}^1$ , different from our original basis  $|i\rangle$ . The new basis vectors can be expressed in terms of the old ones as  $|\alpha\rangle = |i\rangle \langle i|\alpha\rangle$  (with the Einstein summation convention understood). Since the  $a_\alpha^+$  operator acts by adding the particle in the  $\alpha$ -state and the state  $|\alpha\rangle$  is the specific superposition of the states  $|i\rangle$ , the  $a_\alpha^+$  creation operator has to be the same linear combination of the  $a_i^+$  creation operators

$$a_\alpha^+ = \sum_i \langle i|\alpha\rangle a_i^+ \quad a_\alpha = \sum_i \langle \alpha|i\rangle a_i$$

(the relation for the annihilation operators was obtained simply by hermitian conjugation). These relations become handy whenever a need arises for a switch between different bases.

Another point worth discussion is that of continuous bases. Let us recall that the generalized basis vectors  $|\vec{x}\rangle$  or  $|\vec{p}\rangle$  are not elements of the 1-particle Hilbert space, since they are not properly normalized. The generalized normalization condition for the orthonormal  $x$ -basis reads  $\langle \vec{x}|\vec{x}'\rangle = \delta^3(\vec{x} - \vec{x}')$  and any vector  $|\psi\rangle$  from  $\mathcal{H}^1$  can be written as  $|\psi\rangle = \int d^3x |\vec{x}\rangle \langle \vec{x}|\psi\rangle$ . All the relations valid for discrete orthonormal bases hold also for continuous orthonormal bases after the Kronecker deltas are replaced by Dirac deltas and sums by integrals

$$\delta_{ij} \longrightarrow \delta^3(\vec{x} - \vec{x}') \quad \sum_i \longrightarrow \int d^3x$$

The basic relations for the creation and annihilation operators in the  $x$ -representation are

- $a_{\vec{x}}^+ = a_{\vec{x}}^\dagger$  i.e.  $a_{\vec{x}}^+$  and  $a_{\vec{x}}$  are Hermitian conjugated
- for normalized states from the Fock space  $a_{\vec{x}}^+ a_{\vec{x}}$  is not the operator of number of particles with the position  $\vec{x}$ , but rather the operator of density of particles at position  $\vec{x}$  (consequently  $\int d^3x a_{\vec{x}}^+ a_{\vec{x}}$  is the operator of the overall number of particles)
- $[a_{\vec{x}}, a_{\vec{x}'}^+]_{\mp} = \delta^3(\vec{x} - \vec{x}') \quad [a_{\vec{x}}, a_{\vec{x}'}]_{\mp} = [a_{\vec{x}}^+, a_{\vec{x}'}^+]_{\mp} = 0$

The important relations between the creation and annihilation operators in the  $x$ -representation and  $p$ -representations are just continuous versions of the discrete relations given above

$$a_{\vec{p}}^+ = \int d^3x \langle \vec{x}|\vec{p}\rangle a_{\vec{x}}^+ \quad a_{\vec{p}} = \int d^3x \langle \vec{p}|\vec{x}\rangle a_{\vec{x}}$$

where

$$\langle \vec{x}|\vec{p}\rangle = \frac{1}{(2\pi\hbar)^{3/2}} e^{i\vec{p}\cdot\vec{x}/\hbar}$$

for orthonormal²⁸  $p$ -representation basis, i.e. for  $\langle \vec{p}|\vec{p}'\rangle = \delta^3(\vec{p} - \vec{p}')$ . For this basis the relations for the operators  $a_{\vec{p}}^+$ ,  $a_{\vec{p}}$  are completely analogous to the above relations for  $a_{\vec{x}}^+$ ,  $a_{\vec{x}}$ .

²⁸Let us remark that there is a quite common habit to use a specific unnormalized basis in the  $p$ -representation, namely the one where  $\langle \vec{p}|\vec{p}'\rangle = (2\pi\hbar)^3 \delta^3(\vec{p} - \vec{p}')$ . For this basis  $\langle \vec{x}|\vec{p}\rangle = e^{i\vec{p}\cdot\vec{x}/\hbar}$ , the basic (anti)commutation relation reads  $[a(\vec{p}), a^+(\vec{p}')]_{\mp} = (2\pi\hbar)^3 \delta^3(\vec{p} - \vec{p}')$  and the operator of density of particles with the momentum  $\vec{p}$  is  $(2\pi\hbar)^{-3} a^+(\vec{p}) a(\vec{p})$ .

**Remark:** Orthonormality of the basis  $|i\rangle$  in the 1-particle Hilbert space  $\mathcal{H}^1$  played a crucial role in the definition of the specific non-normalized orthogonal basis in the Fock space and in the definition of the creation and annihilation operators. Important features of these operators were consequences of the specific normalization of this Fock space basis. So why should anyone use unnormalized basis in  $\mathcal{H}^1$ ?

The point is that, as we have mentioned several times already, the  $a^+(\vec{p})$  and  $a(\vec{p})$  operators are usually introduced via the so-called canonical quantization, where the starting point is some classical theory. At the classical level, the Fourier transformation is involved, bringing the function  $e^{i\vec{p}\cdot\vec{x}}$  into the game. Now the notoriously known factor of  $(2\pi)^3$  can be used at different places in the definition of the Fourier transformation. And the commonly used choice leads, after quantization, to the non-unit normalization of the basis vectors in the p-representation.

**Remark:** When speaking about different bases in the Fock space, yet another issue should be mentioned. When dealing with various types of particles, one needs a Fock space which contains the Fock spaces of all particle species under consideration. The obvious first choice is the direct product of the corresponding Fock spaces, e.g.  $H = H_A \otimes H_B \otimes H_C$ . In such a case any creation/annihilation operator for one particle type commutes with any c/a operator for any other particle type. Sometimes, however, different particle species may be viewed just as different states of the same particle (due to isospin, eightfold way, etc. symmetries). If so, it is clearly favorable to have a basis and the corresponding (anti)commutation rules which do not need a radical modification with every change of viewpoint. This is achieved by the appropriate choice of the (anti-)symmetrized subspace of the direct product of some of the Fock subspaces, i.e. by the appropriate (anti-)symmetrization of bases of these subspaces, leading to change of some commutation rules by anti-commutation ones.

**Remark:** On top of the creation and annihilation operators, one can encounter yet another – completely different – set of similar operators. The point is that the basis  $|i, j, \dots\rangle$  (or  $|n_1, n_2, \dots\rangle$  in the occupation number formalism), which arises from a particular basis  $|i\rangle$  of the 1-particle Hilbert space, is perhaps the most natural, but not the only reasonable basis in the Fock space. Actually, any complete set of (physically relevant) commuting operators defines some (relevant) basis. (From this point of view, the basis  $|n_1, n_2, \dots\rangle$  is just the basis of eigenvectors of the occupation number operators.)

If the eigenvalues of a complete system of commuting operators are discrete and bounded from below, then one can label both eigenvalues and eigenvectors by natural numbers. In such a case, the basis defined by the considered system of operators looks like  $|N_1, N_2, \dots\rangle$ , and for a basis of this type we can define the so-called raising and lowering operators, just as we have defined the creation and annihilation operators:  $A_i^+$  ( $A_i$ ) raises (lowers) the quantum number  $N_i$  by one.

Of a special interest are the cases when the Hamiltonian can be written as a sum of two terms, one of which has eigenvectors  $|N_1, N_2, \dots\rangle$  with eigenvalues  $E_1 N_1 + E_2 N_2 + \dots$  and the second one can be understood as a small perturbation. If so, the system formally looks like an almost ideal gas (see the next section) made of a new type of particles (created by the  $A_i^+$  operators from the state in which all the  $N_i$  vanish). These formal particles are not to be mistaken for the original particles, which the system consists of.

It may come as a kind of surprise that such formal particles do appear frequently in many-body systems. They are called elementary excitations and they come in great variety (phonons, plasmons, magnons, etc.). Their relation to the original particles is more or less known as the result of either detailed calculations, or an educated guess, or some combination of the two. The description of the system is, as a rule, much simpler in terms of the elementary excitations than in terms of the original particles. This explains the wide use of the elementary excitations language by both theorists and experimentalists.

### 1.2.2 Important operators expressed in terms of $a_i^+, a_i$

As already announced, any linear operator in the Fock space can be written as a polynomial (perhaps infinite) in creation and annihilation operators. As interesting as this general statement may sound, the particular examples are even more interesting and very important in practice. We will therefore start with the examples and return to the general statement only later on.

#### Hamiltonian of a system of non-interacting particles

Let us consider non-interacting particles (ideal gas) in an external classical field with a potential energy  $U(x)$ . The most suitable choice of basis in the 1-particle Hilbert space is the set of eigenstates of the 1-particle Hamiltonian  $\hat{p}^2/2m + U(x)$ , i.e. the states  $|i\rangle$  satisfying

$$\left( \frac{1}{2m} \hat{p}^2 + U(x) \right) |i\rangle = E_i |i\rangle$$

By this choice, the standard basis of the whole Fock space is determined, namely  $|0\rangle$ ,  $|i\rangle$ ,  $|i, j\rangle$ ,  $|i, j, k\rangle$ , etc. And since the particles do not interact, each of these basis states has a sharp value of energy, namely 0,  $E_i$ ,  $E_i + E_j$ ,  $E_i + E_j + E_k$ , etc., respectively. The Hamiltonian of the system with any number of particles is the linear operator with these eigenvectors and these eigenvalues. It is very easy to guess such an operator, namely  $H_0 = \sum_i E_i \hat{n}_i$ , where  $\hat{n}_i$  is the operator of number of particles in the  $i$ -th state. And since we know how to express  $\hat{n}_i$  in terms of the creation and annihilation operators, we are done

$$H_0 = \sum_i E_i a_i^+ a_i$$

- If, for any reason, we would need to express  $H_0$  in terms of another set of creation and annihilation operators  $a_\alpha^+ = \sum_i \langle i|\alpha\rangle a_i^+$  and  $a_\alpha = \sum_i \langle \alpha|i\rangle a_i$ , it is straightforward to do so:  $H_0 = \sum_{\alpha, \beta} E_{\alpha\beta} a_\alpha^+ a_\beta$  where  $E_{\alpha\beta} = \sum_i E_i \langle \alpha|i\rangle \langle i|\beta\rangle$ .
- If one has a continuous quantum number  $q$ , rather than the discrete index  $i$ , then (as we have already discussed) the sum  $\sum_i$  is replaced by the integral  $\int dq$ :  $H_0 = \int dq E(q) a_q^+ a_q$ . Another change is that any Kronecker  $\delta_{ij}$  is replaced by the Dirac delta  $\delta(q - q')$ .

Free particles. 1-particle states labeled by the momentum  $\vec{p}$ , with  $E(\vec{p}) = \frac{p^2}{2m}$

$$H_0 = \int d^3p \frac{p^2}{2m} a_{\vec{p}}^+ a_{\vec{p}}$$

Periodic external field (the 0-th approximation for electrons in solids). Bloch theorem: 1-particle states are labeled by the level  $n$ , the quasi-momentum  $\vec{k}$ , and the spin  $\sigma$ . The energy  $\varepsilon_n(\vec{k})$  depends on details of the periodic field

$$H_0 = \sum_{n, \sigma} \int d^3k \varepsilon_n(\vec{k}) a_{n, \vec{k}, \sigma}^+ a_{n, \vec{k}, \sigma}$$

Spherically symmetric external field (the 0-th approximation for electrons in atoms and nuclei). 1-particle states are labeled by the quantum numbers  $n, l, m, \sigma$ . The energy  $E_{n, l}$  depends on details of the field

$$H_0 = \sum_{n, l, m, \sigma} E_{n, l} a_{n, l, m, \sigma}^+ a_{n, l, m, \sigma}$$

**Remark:** The ideal gas approximation is very popular for electrons in atoms, molecules and solids. At the first sight, however, it looks like a rather poor approximation. The dominant (Coulomb) interaction between electrons is enormous at atomic scale and cannot be neglected in any decent approach.

But there is no mystery involved, the ideal gas approximation used for electrons does not neglect the Coulomb interaction. The point is that the external field for the electron ideal gas contains not only the Coulomb field of positively charged nuclei, but also some kind of mean field of all negatively charged electrons. This mean field is usually given by the Hartree-Fock approximation. The corner-stone of this approximation is a restriction on electron states taken into consideration: only the direct products of single electron states are accounted for. In this restricted set of states one looks for what in some sense is the best approximation to the stationary states. This leads to the specific integro-differential equation for the 1-electron states and corresponding energies, which is then solved iteratively.²⁹ The creation and annihilation operators for these Hartree-Fock states and the corresponding energies then enter the electron ideal gas Hamiltonian.

**Remark:** The ground state of a fermionic system in the Hartree-Fock approximation (the ideal gas approximation with 1-particle states and energies given by the Hartree-Fock equation) is quite simple: all the 1-particle states with energies below some boundary energy, the so-called Fermi energy  $\varepsilon_F$ , are occupied, while all the states with energies above  $\varepsilon_F$  are free. The Fermi energy depends, of course, on the number of particles in the system.

In solids, the 1-particle Hartree-Fock states are characterized by  $(n, \vec{k}, \sigma)$  (level, quasi-momentum, spin). The 1-particle  $n$ -th level Hartree-Fock energy is, as a rule, an ascending function of  $k^2$  in any direction of  $\vec{k}$ . In any direction, therefore, there exists the level  $n$  and the vector  $\vec{k}_F(\varphi, \vartheta)$  for which  $\varepsilon_n(\vec{k}_F) = \varepsilon_F$ . The endpoints of vectors  $\vec{k}_F(\varphi, \vartheta)$  form a surface, called the Fermi surface. In the many-body ground state, the 1-particle states beneath (above) the Fermi surface are occupied (free).

It turns out that for a great variety of phenomena in solids, only the low excited states of the electron system are involved. They differ from the ground state by having a few 1-particle states above the Fermi surface occupied. The particular form of the Fermi surface therefore determines many macroscopic properties of the material under consideration. For this reason the knowledge of the Fermi surface is very important in the solid state physics.

**Remark:** The ideal gas of fermions is frequently treated by means of a famous formal trick known as the electron-hole formalism. The ground state of the  $N$  fermion ideal gas is called the Fermi vacuum, and denoted by  $|0_F\rangle$ . For  $i \leq N$  one defines new operators  $b_i^+ = a_i$  and  $b_i = a_i^+$ . The original  $a_i^+$  and  $a_i$  operators are taken into account only for  $i > N$ .

Both  $a$ - and  $b$ -operators satisfy the commutation relations, and both  $b_i$  ( $i \leq N$ ) and  $a_i$  ( $i > N$ ) annihilate the Fermi vacuum (indeed,  $b_i |0_F\rangle = 0$  because of anti-symmetry of fermion states, i.e. because of the Pauli exclusive principle). So, formally we have two types of particles, the holes and the new electrons, created from the Fermi vacuum by  $b_i^+$  and  $a_i^+$  respectively. The Hamiltonian reads  $H_0 = \sum_{i \leq N} E_i b_i^+ b_i + \sum_{i > N} E_i a_i^+ a_i = \sum_{i \leq N} E_i - \sum_{i \leq N} E_i b_i^+ b_i + \sum_{i > N} E_i a_i^+ a_i$ . The popular interpretation of the minus sign: the holes have negative energy.

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²⁹For details consult any reasonable textbook on QM or solid state physics, or for a very concise introduction perhaps the Appendix ??.

### Hamiltonian of a system of particles with a pair interaction

Perhaps the most important interaction to be added to the previous case of the ideal gas is the pair interaction, i.e. an interaction characterized by a potential energy of pairs of particles (most of applications in the solid state, atomic and nuclear physics involve such an interaction). In this case, the most suitable choice of basis in the 1-particle Hilbert space is the  $x$ -representation  $|\vec{x}\rangle$ , since the 2-particle states  $|\vec{x}, \vec{y}\rangle$  have a sharp value of the pair potential energy  $V(\vec{x}, \vec{y})$ .

Due to the fact that we are dealing with the pair interaction, the 3-particle state  $|\vec{x}_1, \vec{x}_2, \vec{x}_3\rangle$  does also have the sharp value of the potential energy, namely  $V(\vec{x}_1, \vec{x}_2) + V(\vec{x}_1, \vec{x}_3) + V(\vec{x}_2, \vec{x}_3)$ , and the same holds for other multiparticle states (this, in fact, is the definition of the pair interaction).

What is the potential energy of the state with  $n(\vec{x}_i)$  particles at the position  $\vec{x}_i$ , where  $i = 1, 2, \dots$ ? The number of pairs contributing by  $V(\vec{x}_i, \vec{x}_j)$  is  $\frac{1}{2}n_{\vec{x}_i}n_{\vec{x}_j}$  for  $i \neq j$ , by which we understand also  $\vec{x}_i \neq \vec{x}_j$  (the  $\frac{1}{2}$  is there to avoid double-counting). For  $i = j$  there is a subtlety involved. One has to include the potential energy of a particle with all other particles sharing the same position, but not with itself (a particle with itself does not constitute a pair). The number of pairs contributing by  $V(\vec{x}_i, \vec{x}_i)$  is therefore  $\frac{1}{2}n_{\vec{x}_i}(n_{\vec{x}_i} - 1)$ . This makes the total potential energy in the state under consideration equal to  $\frac{1}{2}\sum_{i,j} V(\vec{x}_i, \vec{x}_j)n_{\vec{x}_i}n_{\vec{x}_j} - \frac{1}{2}\sum_i V(\vec{x}_i, \vec{x}_i)n_{\vec{x}_i}$ .

Using the same logic as in the case of the ideal gas, it is now easy to write down the operator of the total potential energy in terms of operators  $\hat{n}_{\vec{x}} = a_{\vec{x}}^+ a_{\vec{x}}$ . Using the commutation relations for the creation and annihilation operators the resulting expression can be simplified to the form³⁰

$$H_{\text{pair}} = \frac{1}{2} \int d^3x d^3y V(\vec{x}, \vec{y}) a_{\vec{x}}^+ a_{\vec{y}}^+ a_{\vec{y}} a_{\vec{x}}$$

Note the order of the creation and annihilation operators, which is mandatory. It embodies the above mentioned subtlety.

As we have seen before, the  $x$ -representation is usually not the most suitable for the ideal gas Hamiltonian. To have the complete Hamiltonian of a system with the pair interaction presented in a single representation, it is useful to rewrite the potential energy operator  $H_{\text{pair}}$  in the other representation.

Free particles. All one needs is  $a_{\vec{x}} = \int d^3p \langle \vec{x} | \vec{p} \rangle a_{\vec{p}} = \int \frac{d^3p}{\sqrt{(2\pi\hbar)^3}} e^{i\vec{p}\cdot\vec{x}/\hbar} a_{\vec{p}}$

$$H_{\text{pair}} = \frac{1}{2} \int d^3p_1 d^3p_2 d^3p_3 d^3p_4 V(\vec{p}_1, \vec{p}_2, \vec{p}_3, \vec{p}_4) a_{\vec{p}_1}^+ a_{\vec{p}_2}^+ a_{\vec{p}_3} a_{\vec{p}_4}$$

$$V(\vec{p}_1, \vec{p}_2, \vec{p}_3, \vec{p}_4) = \int \frac{d^3x}{(2\pi\hbar)^3} \frac{d^3y}{(2\pi\hbar)^3} V(\vec{x}, \vec{y}) \exp \frac{i(\vec{p}_4 - \vec{p}_1) \cdot \vec{x}}{\hbar} \exp \frac{i(\vec{p}_3 - \vec{p}_2) \cdot \vec{y}}{\hbar}$$

Periodic external field. Replace the plane waves  $\langle \vec{x} | \vec{p} \rangle$  by the Bloch functions  $\langle \vec{x} | n, \vec{k} \rangle = u_n(\vec{k}) e^{i\vec{k}\cdot\vec{x}}$ .

Spherically symmetric external field. Replace the plane waves  $\langle \vec{x} | \vec{p} \rangle$  by the product of the radial Schrödinger equation solutions and spherical harmonics  $\langle \vec{x} | n, l, m \rangle = R_{nl}(r) Y_{lm}(\varphi, \vartheta)$ .

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³⁰  $U = \frac{1}{2} \int d^3x d^3y V(\vec{x}, \vec{y}) a_{\vec{x}}^+ a_{\vec{x}} a_{\vec{y}}^+ a_{\vec{y}} - \frac{1}{2} \int d^3x V(\vec{x}, \vec{x}) a_{\vec{x}}^+ a_{\vec{x}}$   
 $= \frac{1}{2} \int d^3x d^3y V(\vec{x}, \vec{y}) a_{\vec{x}}^+ \left( \delta(\vec{x} - \vec{y}) \pm a_{\vec{y}}^+ a_{\vec{x}} \right) a_{\vec{y}} - \frac{1}{2} \int d^3x V(\vec{x}, \vec{x}) a_{\vec{x}}^+ a_{\vec{x}}$   
 $= \pm \frac{1}{2} \int d^3x d^3y V(\vec{x}, \vec{y}) a_{\vec{x}}^+ a_{\vec{y}}^+ a_{\vec{x}} a_{\vec{y}} = \frac{1}{2} \int d^3x d^3y V(\vec{x}, \vec{y}) a_{\vec{x}}^+ a_{\vec{y}}^+ a_{\vec{y}} a_{\vec{x}}$

**Remark:** Even if it is not necessary for our purposes, it is hard to resist the temptation to discuss perhaps the most important pair interaction in the non-relativistic quantum physics, namely the Coulomb interaction. This is of general interest not only because of the vast amount of applications, but also due to the fact that the standard way of dealing with the Coulomb potential in the  $p$ -representation involves a mathematical inconsistency. The way in which this inconsistency is treated is in a sense generic, and therefore quite instructive. In the  $x$ -representation  $V_{\text{Coulomb}}(\vec{x}, \vec{y}) = \frac{e^2}{4\pi} \frac{1}{|\vec{x} - \vec{y}|}$ , i.e. in the  $p$ -representation (which is relevant in the case with no external field)

$$V_{\text{Coulomb}}(\vec{p}_1, \vec{p}_2, \vec{p}_3, \vec{p}_4) = \frac{e^2}{4\pi} \int \frac{d^3x}{(2\pi)^3} \frac{d^3y}{(2\pi)^3} \frac{1}{|\vec{x} - \vec{y}|} e^{i(\vec{p}_4 - \vec{p}_1) \cdot \vec{x}} e^{i(\vec{p}_3 - \vec{p}_2) \cdot \vec{y}}$$

(for the sake of brevity, we use the Heaviside-Lorentz convention in electrodynamics and  $\hbar = 1$  units in QM). This integral, however, is badly divergent. The integrand simply does not drop out fast enough for  $|\vec{x}| \rightarrow \infty$  and  $|\vec{y}| \rightarrow \infty$ .

Instead of giving up the use of the  $p$ -representation for the Coulomb potential energy, it is a common habit to use a dirty trick. It starts by considering the Yukawa (or Debey) potential energy  $V_{\text{Debey}}(\vec{x}, \vec{y}) = \frac{e^2}{4\pi} \frac{1}{|\vec{x} - \vec{y}|} e^{-\mu|\vec{x} - \vec{y}|}$ , for which the  $p$ -representation is well defined and can be evaluated readily³¹

$$V_{\text{Debey}}(\vec{p}_1, \vec{p}_2, \vec{p}_3, \vec{p}_4) = \frac{e^2}{4\pi} \frac{1}{2\pi^2} \frac{1}{\mu^2 + (\vec{p}_4 - \vec{p}_1)^2} \delta(\vec{p}_1 + \vec{p}_2 - \vec{p}_3 - \vec{p}_4)$$

Now comes the dirty part. It is based on two simple (almost trivial) observations: the first is that  $V_{\text{Coulomb}}(\vec{x}, \vec{y}) = \lim_{\mu \rightarrow 0} V_{\text{Debey}}(\vec{x}, \vec{y})$ , and the second is that the limit  $\lim_{\mu \rightarrow 0} V_{\text{Debey}}(\vec{p}_1, \vec{p}_2, \vec{p}_3, \vec{p}_4)$  is well defined. From this, a brave heart can easily conclude that  $V_{\text{Coulomb}}(\vec{p}_1, \vec{p}_2, \vec{p}_3, \vec{p}_4) = \frac{e^2}{8\pi^3} \frac{1}{(\vec{p}_4 - \vec{p}_1)^2} \delta(\vec{p}_1 + \vec{p}_2 - \vec{p}_3 - \vec{p}_4)$ . And, believe it or not, this is indeed what is commonly used as the Coulomb potential energy in the  $p$ -representation.

Needless to say, from the mathematical point of view, this is an awful heresy (called illegal change of order of a limit and an integral). How does it come about that physicists are working happily with something so unlawful?

The most popular answer is that the Debey is nothing else but a screened Coulomb, and that in most systems this is more realistic than the pure Coulomb. This is a reasonable answer, with a slight off-taste of a cheat (the limit  $\mu \rightarrow 0$  convicts us that we are nevertheless interested in the pure Coulomb).

Perhaps a bit more fair answer is this one: For  $\mu$  small enough, one cannot say experimentally the difference between Debey and Coulomb. And the common plausible belief is that measurable outputs should not depend on immeasurable inputs (if this was not typically true, whole science would hardly be possible). If mathematics nevertheless reveals inconsistencies for some values of an immeasurable parameter, one should feel free to choose another value, which allows for mathematically sound treatment.

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³¹For  $\vec{r} = \vec{x} - \vec{y}$ ,  $V_{\text{Yukawa}}(\vec{p}_1, \vec{p}_2, \vec{p}_3, \vec{p}_4) = \frac{e^2}{4\pi} \int \frac{d^3r}{(2\pi)^3} \frac{d^3y}{(2\pi)^3} \frac{1}{r} e^{-\mu r} e^{i(\vec{p}_4 - \vec{p}_1) \cdot \vec{r}} e^{i(\vec{p}_3 - \vec{p}_2 + \vec{p}_4 - \vec{p}_1) \cdot \vec{y}}$   
 $= \frac{e^2}{4\pi} \delta(\vec{p}_1 + \vec{p}_2 - \vec{p}_3 - \vec{p}_4) \int \frac{d^3r}{(2\pi)^3} \frac{e^{-\mu r}}{r} e^{i\vec{q} \cdot \vec{r}}$ , where  $\vec{q} = \vec{p}_4 - \vec{p}_1$ . The remaining integral in the spherical coordinates:  $\frac{1}{(2\pi)^2} \int_0^\infty dr r e^{-\mu r} \int_{-1}^1 d\cos\vartheta e^{iqr\cos\vartheta} = \frac{1}{2\pi^2} \frac{1}{q} \int_0^\infty dr e^{-\mu r} \sin qr$ . For the integral  $I = \int_0^\infty dr e^{-\mu r} \sin qr$  one obtains by double partial integration the relation  $I = \frac{q}{\mu^2} - \frac{q^2}{\mu^2} I$ , and putting everything together, one comes to the quoted result.

### Hamiltonian of a system of unstable particles (and related systems)

Let us consider a system of particles of three types  $A$ ,  $B$  and  $C$ , one of which decays into other two,³² say  $C \rightarrow AB$ . The decay can be understood as the annihilation of the decaying particle and the simultaneous creation of the products. The corresponding interaction Hamiltonian, i.e. the part of the time-evolution generator responsible for this kind of change, is almost self-evident.³³ It should contain the combination  $a_i^+ b_j^+ c_k$ , where the lowercase letters for creation and annihilation operators correspond to the uppercase letters denoting the type of particle, and subscripts specify the states of the particles involved.

The decay is usually allowed for various combinations of the quantum numbers  $i, j, k$ , so the interaction Hamiltonian should assume the form of the sum of all legal alternatives. This is usually written as the sum of all alternatives, each of them multiplied by some factor, which vanishes for the forbidden combinations of quantum numbers:  $\sum_{i,j,k} g_{ijk} a_i^+ b_j^+ c_k$ .

There is still one problem with this candidate for the interaction Hamiltonian: it is not Hermitian. But this is quite easy to take care of, one just adds the Hermitian conjugate operator  $g_{ijk}^* c_k^\dagger b_j a_i$ . So the Hermiticity of the Hamiltonian requires, for any decay, the existence of the reverse process  $AB \rightarrow C$ . All in all

$$H_{\text{int}} = \sum_{i,j,k} g_{ijk} a_i^+ b_j^+ c_k + g_{ijk}^* c_k^\dagger b_j a_i$$

For a Hamiltonian of this type the  $C$  particles need not to be necessary unstable. If the mass of the  $C$  particle is smaller than the masses of  $A$  and  $B$  particles then decay may be kinematically forbidden (due to the momentum  $\delta$ -function in the final formula for the decay rate). Many of the realistic Hamiltonians of this type describe stable particles, in spite of the fact that we have introduced it naturally for unstable particles.

In some cases the particles  $C$  and  $B$  can be identical (even if in different states), while the particle  $A$  is some other particle (e. g. photon). The interaction Hamiltonian is

$$H_{\text{int}} = \sum_{i,j,k} g_{ijk} a_i^+ b_j^+ b_k + g_{ijk}^* b_k^\dagger b_j a_i$$

The states of the particle  $B$  could be those of the electron in the hydrogen atom³⁴, or an electron in a periodic potential (solid state physics) or a free charged particle (Compton scattering).

The factor  $g_{ijk}$  is usually called the coupling constant, although it depends on the quantum numbers  $i, j, k$ . The reason for the name constant is that most of decays are local and translation invariant (they do not vary with changes in position). In the  $x$ -representation the locality means that  $g_{\vec{x},\vec{y},\vec{z}} = g_{\vec{x}} \delta(\vec{x}-\vec{y}) \delta(\vec{x}-\vec{z})$  and translational invariance requires that  $g$  does not depend on  $\vec{x}$

$$H_{\text{int}} = \int d^3x g a_{\vec{x}}^+ b_{\vec{x}}^+ c_{\vec{x}} + g^* c_{\vec{x}}^\dagger b_{\vec{x}} a_{\vec{x}}$$

³²Generalizations to decays with three or more products (or even some more bizarre processes, with more than one particle annihilated) are straightforward.

³³In the previous two cases the form of the Hamiltonian was deduced from the fact that it is the operator of energy. Now we are using another role of the Hamiltonian, namely that it is the generator of time evolution.

³⁴Basic courses of quantum mechanics start with Einstein's photons and culminate with the Schrödinger equation in which photons are not present. Indeed, the Schrödinger equation for the hydrogen atom explains the discrete spectrum treating electromagnetic field (both internal and external) classically. For quantum description of photon emission/absorption, the creation and annihilation operators are needed.

**Remark:** *phonon-phonon interaction*

**Remark:** *electron-phonon interaction*

**Remark:** *electron-photon interaction*

### any linear operator expressed in terms of $a^+, a$

The only purpose of this paragraph is to satisfy a curious reader (if there is any). It will be of no practical importance to us.

First of all, it is very easy to convince oneself that any linear operator can be expressed in terms of creation operators  $a_i^+$ , annihilation operators  $a_i$  and the vacuum projection operator  $|0\rangle\langle 0|$ . Indeed, if  $\hat{A}$  is a linear operator, then

$$\hat{A} = \sum_{\substack{i,j,\dots \\ k,l,\dots}} A_{ij\dots,kl\dots} a_i^+ a_j^+ \dots |0\rangle\langle 0| a_k a_l \dots$$

where  $A_{ij\dots,kl\dots} = \frac{\langle i,j,\dots|\hat{A}|k,l,\dots\rangle}{\langle i,j,\dots|i,j,\dots\rangle\langle k,l,\dots|k,l,\dots\rangle}$ . Proof: both LHS and RHS have the same matrix elements for all combinations of basis vectors (check this).

The only question therefore is how to get rid of  $|0\rangle\langle 0|$ . This is done by induction. First, one expresses the  $\hat{A}$  operator only within the 0-particle subspace  $\mathcal{H}^0$  of the Fock space, where it is nothing else but the multiplication by the constant

$$\hat{A}_0 = \tilde{A}_{0,0} \equiv \langle 0|\hat{A}|0\rangle$$

Then, one expresses the  $\hat{A}_1 = \hat{A} - \hat{A}_0$  operator within the 0- and 1-particle subspace  $\mathcal{H}^0 \oplus \mathcal{H}^1$ . Here one gets (check it)

$$\hat{A}_1 = \tilde{A}_{i,j} a_i^+ a_j + \tilde{A}_{i,0} a_i^+ + \tilde{A}_{0,j} a_j$$

where  $\tilde{A}_{ij} = \langle i|\hat{A} - \hat{A}_0|j\rangle$ ,  $\tilde{A}_{i,0} = \langle i|\hat{A} - \hat{A}_0|0\rangle$  and  $\tilde{A}_{0,j} = \langle 0|\hat{A} - \hat{A}_0|j\rangle$ . If one restricts oneself to  $\mathcal{H}^0 \oplus \mathcal{H}^1$ , then  $\hat{A} = \hat{A}_0 + \hat{A}_1$  (why?). So we have succeeded in writing the operator  $\hat{A}$  in terms of  $a_i^+, a_i$ , even if only in the subspace of the Fock space. This subspace is now expanded to  $\mathcal{H}^0 \oplus \mathcal{H}^1 \oplus \mathcal{H}^2$ , etc.

It may be instructive now to work out the operator  $\hat{A}_2 = \hat{A} - \hat{A}_0 - \hat{A}_1$  within  $\mathcal{H}^0 \oplus \mathcal{H}^1 \oplus \mathcal{H}^2$  in terms of  $a_i^+, a_i$  (try it). We will, however, proceed directly to the general case of  $\hat{A}_n = \hat{A} - \sum_{m=0}^{n-1} \hat{A}_m$  within  $\bigoplus_{m=0}^n \mathcal{H}^m$

$$\begin{aligned} \hat{A}_n &= \sum_{\substack{\text{allowed} \\ \text{combinations}}} \tilde{A}_{ij\dots,kl\dots} a_i^+ a_j^+ \dots a_k a_l \dots \\ \tilde{A}_{ij\dots,kl\dots} &= \frac{\langle i,j,\dots|\hat{A} - \sum_{m=0}^{n-1} \hat{A}_m|k,l,\dots\rangle}{\langle i,j,\dots|i,j,\dots\rangle\langle k,l,\dots|k,l,\dots\rangle} \end{aligned}$$

and the "allowed combinations" are either  $\underbrace{ij\dots}_n, \underbrace{kl\dots}_{m \leq n}$  or  $\underbrace{ij\dots}_{m \leq n}, \underbrace{kl\dots}_n$ .

If restricted to  $\bigoplus_{m=0}^n \mathcal{H}^m$ , then  $\hat{A} = \sum_{m=0}^n \hat{A}_m$ , i.e. we have  $\hat{A}$  expressed in terms of  $a_i^+, a_i$ . To get an expression valid not only in subspaces, one takes

$$\hat{A} = \sum_{m=0}^{\infty} \hat{A}_m$$

### 1.2.3 Calculation of matrix elements — the main trick

One of the most valuable benefits of the use of the creation and annihilation operator formalism is the completely automatous way of matrix elements calculation. The starting point is twofold:

- any ket (bra) vector can be written as a superposition of the basis vectors, which in turn can be obtained by  $a_i^+$  ( $a_i$ ) operators acting on  $|0\rangle$
- any linear operator can be written as a linear combination of products of the  $a_i^+$  and  $a_i$  operators

Consequently, any matrix element of a linear operator is equal to some linear combination of the vacuum expectation values (VEVs) of the products of the creation and annihilation operators.

Some of the VEVs are very easy to calculate, namely those in which the last (first) operator in the product is the annihilation (creation) one. Indeed, due to  $a_i|0\rangle = 0$  and  $\langle 0|a_i^+ = 0$ , any such VEV vanishes. Other VEVs are easily brought to the previous form, one just has to use the (anti)commutation relations  $[a_i, a_j^\pm]_\mp = \delta_{ij}$  to push the annihilation (creation) operators to the right (left). By repeated use of the (anti)commutation relations, the original VEV is brought to the sum of scalar products  $\langle 0|0\rangle$  multiplied by pure numbers, and the VEVs vanishing because of  $\langle 0|a_i^+ = 0$  or  $a_i|0\rangle = 0$ . An example is perhaps more instructive than a general exposition.

**Example:** Let us consider a decay-like Hamiltonian for just one type of particles  $H_{\text{decay}} = \sum_{i,j,k} g_{ijk}(a_i^+ a_j^+ a_k + a_k^+ a_j a_i)$  (e.g. phonons, as well as gluons, enjoy this kind of interaction). Note that the coupling "constant" is real  $g_{ijk} = g_{ijk}^*$ . And let us say we want to calculate  $\langle l|H_{\text{decay}}|m, n\rangle$ . First, one writes

$$\langle l|H_{\text{decay}}|m, n\rangle = \sum_{i,j,k} g_{ijk} (\langle 0|a_l a_i^+ a_j^+ a_k a_m^+ a_n^+|0\rangle + \langle 0|a_l a_k^+ a_j a_i a_m^+ a_n^+|0\rangle)$$

Then one starts to reshuffle the operators. Take, e.g., the first two and use  $a_l a_i^+ = \delta_{li} \pm a_i^+ a_l$  (or with  $i$  replaced by  $k$  in the second term), to obtain

$$\begin{aligned} \langle l|H_{\text{decay}}|m, n\rangle = \sum_{i,j,k} g_{ijk} (\delta_{li} \langle 0|a_j^+ a_k a_m^+ a_n^+|0\rangle \pm \langle 0|a_i^+ a_l a_j^+ a_k a_m^+ a_n^+|0\rangle \\ + \delta_{lk} \langle 0|a_j a_i a_m^+ a_n^+|0\rangle \pm \langle 0|a_k^+ a_l a_j a_i a_m^+ a_n^+|0\rangle) \end{aligned}$$

Three of the four terms have  $a^+$  next to  $\langle 0|$ , and consequently they vanish. In the remaining term (the third one) one continues with reshuffling

$$\begin{aligned} \langle l|H_{\text{decay}}|m, n\rangle &= \sum_{i,j,k} g_{ijk} \delta_{lk} (\delta_{im} \langle 0|a_j a_n^+|0\rangle \pm \langle 0|a_j a_m^+ a_i a_n^+|0\rangle) \\ &= \sum_{i,j,k} g_{ijk} \delta_{lk} (\delta_{im} \delta_{jn} \pm \delta_{jm} \langle 0|a_i a_n^+|0\rangle + 0) \\ &= \sum_{i,j,k} g_{ijk} \delta_{lk} (\delta_{im} \delta_{jn} \pm \delta_{jm} \delta_{in}) = g_{mnl} \pm g_{nml} \end{aligned}$$

The result could be seen directly from the beginning. The point was not to obtain this particular result, but rather to illustrate the general procedure. It should be clear from the example, that however complicated the operator and the states (between which it is sandwiched) are, the calculation proceeds in the same way: one just reshuffles the creation and annihilation operators.

The example has demonstrated an important common feature of this type of calculations: after all the rubbish vanishes, what remains are just products of deltas (Kronecker or Dirac for discrete or continuous cases respectively), each delta originating from some pair of  $a a^+$ . This enables a short-cut in the whole procedure, namely to take into account only those terms in which all  $a$  and  $a^+$  operators can be organized (without leftovers) in the pairs  $a a^+$  (in this order!), and to assign the appropriate  $\delta$  to every such pair.

This is usually done within the "clip" notation, like e.g.  $\overbrace{\dots a_i \dots a_j^+}^{\text{clip}} \dots$ , which tells us that  $a_i$  is paired with  $a_j^+$ . The factor corresponding to this particular clip is therefore  $\delta_{ij}$ . In the case of fermions one has to keep track of signs. The reader may try to convince him/herself that the rule is: every pair of clips biting into each other, generates the minus sign for fermions.

**Example:** *The same example as above, now using the clip short-cut.*

$$\langle l | H_{\text{decay}} | m, n \rangle = \sum_{i,j,k} g_{ijk} (\langle 0 | a_l a_i^+ a_j^+ a_k a_m^+ a_n^+ | 0 \rangle + \langle 0 | a_l a_k^+ a_j a_i a_m^+ a_n^+ | 0 \rangle)$$

The first term cannot be organized (without leftovers) in pairs of  $aa^+$ , so it does not contribute. As to the rest, one has

$$\langle 0 | a_l a_k^+ a_j a_i a_m^+ a_n^+ | 0 \rangle = \langle 0 | \overbrace{a_l a_k^+} \overbrace{a_j a_i a_m^+ a_n^+} | 0 \rangle + \langle 0 | \overbrace{a_l a_k^+} \overbrace{a_j a_i a_m^+ a_n^+} | 0 \rangle = \delta_{lk} \delta_{jn} \delta_{im} \pm \delta_{lk} \delta_{jm} \delta_{in}$$

leading immediately to the same result as before ( $g_{mnl} \pm g_{nml}$ ).

The common habit is to make the short-cut even shorter. Instead of writing the clips above or under the corresponding operators, one draws just the clips and then assigns the corresponding factor to the whole picture. In this comics-like formalism our matrix element would become

$$\begin{array}{ccc} l & \text{---} & k \\ j & \text{---} & n \\ i & \text{---} & m \end{array} \quad \pm \quad \begin{array}{ccc} l & \text{---} & k \\ j & \text{---} & m \\ i & \text{---} & n \end{array}$$

If the interaction is local, the picture is changed slightly. Local interactions contain products of operators in the same position, e.g.  $a_{\vec{x}}^+ b_{\vec{x}}^+ c_{\vec{x}}$ , which in our discrete case would correspond to  $H_{\text{decay}} = \sum_i g(a_i^+ a_i^+ a_i + a_i^+ a_i a_i)$ . For fermions this Hamiltonian vanishes (why?), for bosons result becomes  $g \sum_i (\delta_{li} \delta_{in} \delta_{im} + \delta_{li} \delta_{im} \delta_{in})$  and the above picture is changed to

$$\begin{array}{c} m \\ \diagup \\ l \text{ --- } i \\ \diagdown \\ n \end{array} \quad + \quad \begin{array}{c} n \\ \diagup \\ l \text{ --- } i \\ \diagdown \\ m \end{array}$$

**Exercise: (a useful one)** For bosonic particles with  $H_{\text{decay}} = \sum_i g(a_i^+ a_i^+ a_i + a_i^+ a_i a_i)$  calculate  $\langle k, l | H_{\text{decay}} H_{\text{decay}} | m, n \rangle$  and draw the corresponding pictures.

Answer:  $12g^2$  for  $k = l = m = n$  (and 0 otherwise).  
The pictures corresponding to the matrix element are (contributing 4 times each).

$$\begin{array}{ccc} \begin{array}{c} k \\ \diagup \\ l \text{ --- } i \\ \diagdown \\ n \end{array} & \begin{array}{c} m \\ \diagup \\ l \text{ --- } i \\ \diagdown \\ n \end{array} & \begin{array}{c} k \\ \diagup \\ l \text{ --- } i \\ \diagdown \\ n \end{array} \end{array}$$

### Feynman diagrams – a comics version of a perturbation theory

The pictures from the exercise at the end of the previous paragraph may suggest some relation to the Feynman diagrams and indeed they are closely related. In this subsection (which can be skipped safely) we will demonstrate that in a theory with the interaction Hamiltonian written in terms of creation and annihilation operators various terms of a perturbation series can be represented by such diagrams. We will not derive the Feynman rules presented in Conclusions yet (this will be achieved only later on), but the basic idea should become clear already now.

One can illustrate the whole procedure on a simple example of time-independent perturbation theory, where eigenvalues  $E_n$  and eigenstates  $|\psi_n\rangle$  of a complete Hamiltonian  $H = H_0 + \alpha H'$  are expressed in terms of eigenvalues  $\mathcal{E}_n$  and eigenstates  $|\varphi_n\rangle$  of the unperturbed  $H_0$ . Let us recall that this is achieved by expanding the  $E_n$  and  $|\psi_n\rangle$  in powers of  $\alpha$ :  $E_n = \mathcal{E}_n + \sum_{k=1}^{\infty} \alpha^k E_n^{(k)}$  and  $|\psi_n\rangle = |\varphi_n\rangle + \sum_{k=1}^{\infty} \alpha^k |\psi_n^{(k)}\rangle$ , where  $H_0 |\varphi_n\rangle = \mathcal{E}_n |\varphi_n\rangle$  and  $\langle \varphi_n | \psi_n^{(k)} \rangle = 0$ . Comparing coefficients of various powers of  $\alpha$  in the equation  $(H_0 + \alpha H') |\psi_n\rangle = E_n |\psi_n\rangle$  one obtains explicit formulae for the expansion coefficients. The lowest order results are well known from any textbook on quantum mechanics, in non-degenerate case one gets

$$E_n^{(1)} = \langle \varphi_n | H' | \varphi_n \rangle \quad E_n^{(2)} = \sum_{m \neq n} \frac{\langle \varphi_n | H' | \varphi_m \rangle \langle \varphi_m | H' | \varphi_n \rangle}{\mathcal{E}_n - \mathcal{E}_m}$$

The higher orders are more involved, e.g.

$$E_n^{(3)} = \sum_{m, m' \neq n} \frac{\langle \varphi_n | H' | \varphi_m \rangle \langle \varphi_m | H' | \varphi_{m'} \rangle \langle \varphi_{m'} | H' | \varphi_n \rangle}{(\mathcal{E}_n - \mathcal{E}_m)(\mathcal{E}_n - \mathcal{E}_{m'})} + \dots$$

where ellipses stand for additional terms, which have a similar structure (product of the interaction Hamiltonians sandwiched between various states in the numerator and product of energy differences in the denominator) and their complexity increases with increasing order.

Let us consider, as an example, a system of free non-relativistic bosons with a local decay-like interaction (with a real  $g$ ). The unperturbed and the perturbation Hamiltonians are

$$H_0 = \int d^3p \frac{p^2}{2m} a_{\vec{p}}^+ a_{\vec{p}} \quad H' = g \int d^3x (a_{\vec{x}}^+ a_{\vec{x}}^+ a_{\vec{x}} + a_{\vec{x}}^+ a_{\vec{x}} a_{\vec{x}})$$

respectively. Since the eigenstates of the  $H_0$  are the vectors  $|\vec{p}\rangle$ , it is convenient to rewrite  $H'$  into the  $p$ -representation, using the relations  $a_{\vec{x}} = \int \frac{d^3k}{(2\pi\hbar)^{3/2}} e^{i\vec{k}\cdot\vec{x}/\hbar} a_{\vec{k}}$  and  $a_{\vec{x}}^+ = \int \frac{d^3k}{(2\pi\hbar)^{3/2}} e^{-i\vec{k}\cdot\vec{x}/\hbar} a_{\vec{k}}^+$ . After plugging this into  $H'$  and integrating over  $d^3x$  (recall  $\int dx e^{-ikx} = 2\pi\delta(k)$ ) one obtains

$$H' = g \int \frac{d^3k_1}{(2\pi\hbar)^{3/2}} \frac{d^3k_2}{(2\pi\hbar)^{3/2}} \frac{d^3k_3}{(2\pi\hbar)^{3/2}} (2\pi\hbar)^{3/2} \delta(\vec{k}_1 + \vec{k}_2 - \vec{k}_3) a_{\vec{k}_1}^+ a_{\vec{k}_2}^+ a_{\vec{k}_3} + h.c.$$

For such a  $H'$  the only non-vanishing matrix elements are those between states in which number of particles differ precisely by one. The first order correction to energy of one-particle state  $E_{\vec{p}}^{(1)} = \langle \vec{p} | H' | \vec{p} \rangle$  is therefore zero. In the second order correction one has non-vanishing matrix elements  $\langle \vec{p} | H' | \varphi_m \rangle$  for two-particle states  $|\varphi_m\rangle = |\vec{p}', \vec{p}''\rangle$ , i.e.

$$E_{\vec{p}}^{(2)} = \int d^3p' d^3p'' \frac{\langle \vec{p} | H' | \vec{p}', \vec{p}'' \rangle \langle \vec{p}', \vec{p}'' | H' | \vec{p} \rangle}{(p^2 - p'^2 - p''^2)/2m}.$$

Now using the technique of the previous subsection one can represent the matrix elements in the numerator of  $E_p^{(2)}$  by two pictures, namely  $\text{---}\langle$  and  $\text{---}\rangle$ . And since the RHS two-particle state of the first picture is the same as the LHS two-particle state of the second picture, one can draw their product as  $\text{---}\bigcirc\text{---}$ . Now just like in the previous subsection one gets

$$\langle \vec{p} | a_{\vec{k}_1}^+ a_{\vec{k}_2}^+ a_{\vec{k}_3} + h.c. | \vec{p}', \vec{p}'' \rangle = \delta(\vec{p} - \vec{k}_3) \delta(\vec{p}' - \vec{k}_2) \delta(\vec{p}'' - \vec{k}_1) \pm \delta(\vec{p} - \vec{k}_3) \delta(\vec{p}' - \vec{k}_1) \delta(\vec{p}'' - \vec{k}_2)$$

and so for bosons

$$\langle \vec{p} | H' | \vec{p}', \vec{p}'' \rangle = \frac{2g}{(2\pi\hbar)^3} \delta(\vec{p}' + \vec{p}'' - \vec{p})$$

while for fermions this matrix element vanishes. Our expression for the second order correction to the energy of bosons (not only the numerator, but rather the whole second order correction) can be therefore written as the diagram

$$E_n^{(2)} = \text{---}\bigcirc\text{---}$$

with the following rules³⁵

- To every internal line assign the factor  $\int d^3p$
- To every vertex assign the factor  $\frac{2g}{(2\pi\hbar)^3} \delta(\vec{p}' + \vec{p}'' - \vec{p})$
- To every intermediate state  $|\varphi_m\rangle$  assign the factor  $\frac{1}{\varepsilon_n - \varepsilon_m}$

The intermediate states are the states of several free particles (with specific momenta) represented by internal lines of the diagram. When going from left to right, every vertex changes the number of particles, i.e. the intermediate state is changed and the corresponding energy denominator should be added.

The point of the diagrams and the rules is that they work in the same way also for higher order corrections, e.g. with these rules one can easily write (draw)

$$E_n^{(4)} = \text{---}\bigcirc\bigcirc\text{---} + \text{---}\bigcirc\bigcirc\text{---} + \text{---}\bigcirc\bigcirc\text{---} + \dots$$

We are not going to elaborate further and to derive the rules in their full complexity (e.g. we are not going to formulate the rules for terms hidden in ellipses). The purpose of this paragraph was just to give a basic taste of how do the Feynman diagrams and rules emerge in a quantum theory. All the details are to be discussed only when a specific perturbation theory within the relativistic quantum theory is developed in the next chapter.

³⁵Note that these diagrams are not exactly the ones described in Conclusions. They represent different quantities (the energy eigenvalues, not the scattering amplitude) and the rules are also different (the factors for intermediate states, not for internal lines). But what they do have in common is that they are just pictorial representations of various terms in perturbative expansion of some quantity in some version of the perturbation theory.

**Remark:** It is probably worth mentioning that there exists an equivalent, but slightly different version of the perturbation theory for energy eigenvalues, in which complexity of terms does not increase with the increasing order. It is known as the *Brillouin–Wigner perturbation theory* (while the standard version notoriously known from textbooks is called the *Rayleigh–Schrödinger perturbation theory*). In the BW version one obtains equally simple expressions in all orders (for derivation see the next remark)

$$E_n^{(k)} = \sum_{m_1, \dots, m_{k-1} \neq n} \frac{\langle \varphi_n | H' | \varphi_{m_1} \rangle \dots \langle \varphi_{m_{k-1}} | H' | \varphi_n \rangle}{(E_n - \mathcal{E}_{m_1}) \dots (E_n - \mathcal{E}_{m_{k-1}})}$$

Note the presence of  $E_n$  (instead of  $\mathcal{E}_n$ ) on the RHS of the last relation. Because of this, the relation is only an implicit one and has to be solved (either iteratively or by expansion of  $E_n$  in powers of  $\alpha$ ) to get the explicit result for  $E_n^{(k)}$  (which is, as it should be, equal to the standard version of the perturbation theory). Due to its simpler structure the BW version of the perturbation theory is better suited for the Feynman diagrammatical representation than the RS version. Reason: no ellipses in the BW version (the terms corresponding to the ellipses in the RS version can be also represented by Feynman diagrams, but with more complicated rules). Moral: for some versions of the perturbation theory the Feynman diagrams are more suitable than for the others.

**Remark:** For the sake of completeness we will sketch here the derivation of the Brillouin–Wigner perturbation theory (see the previous remark). One possible way is to start with another version of a perturbation theory, namely the one for the particle scattering. This is of interest by itself, because it provides us with yet another example of Feynman diagrams in Quantum mechanics.

In QM textbooks the potential scattering is usually treated by solving the time-independent Schrödinger equation in the  $x$ -representation.³⁶ This, however, is not best suited for the formalism of creation and annihilation operators. Fortunately, the whole idea can be generalized in a relatively easy way. One writes the Schrödinger equation in the form  $(E - H_0) |\psi_l\rangle = \alpha H' |\psi_l\rangle$ , where  $l$  stays for a label (which is continuous in the case of scattering). This equation is solved formally using the inverse operator³⁷  $(E - H_0)^{-1}$ . The inverse operator for  $E - H_0$ , however, does not exist, since the operator  $E - H_0$  has the zero eigenvalue. It is therefore a common habit to consider the operator  $E - H_0 + i\epsilon$  instead (this can be viewed as a generalisation of the  $i\epsilon$  prescription in the complex plane integration for the Green function). The implicit solution of the Schrödinger equation is written as the so-called Lippman-Schwinger equation

$$|\psi\rangle = |\varphi\rangle + (E - H_0 + i\epsilon)^{-1} \alpha H' |\psi\rangle$$

where  $|\varphi\rangle$  is a solution of the homogeneous equation  $(E - H_0) |\varphi\rangle = 0$ .

³⁶A brief reminder: The Schrödinger equation for potential scattering is rewritten as a Helmholtz-like equation  $(E - H_0)\psi(\vec{r}) = \alpha H'\psi(\vec{r})$  with  $H_0 = -\frac{\hbar^2}{2m}\Delta$  and  $H' = U(\vec{r})$ . The solution of this equation is expressed via the Green function  $G_+(\vec{r}, \vec{r}')$  satisfying  $\left(\frac{\hbar^2}{2m}\Delta + E\right)G_+(\vec{r}, \vec{r}') = \delta(\vec{r} - \vec{r}')$  and the "outgoing wave" boundary condition  $G_+(\vec{r}, \vec{0})_{r \rightarrow \infty} \rightarrow \frac{f(\varphi, \vartheta)}{r} e^{ikr}$  where  $E = \frac{\hbar^2 k^2}{2m}$ . The Green function is usually found by Fourier transforming the equation, solving the resulting algebraic equation and backward Fourier transforming the solution with integration in the complex plane, the result is  $G_+(\vec{r}, \vec{r}') = -\frac{1}{4\pi|\vec{r} - \vec{r}'|} e^{i\vec{k} \cdot (\vec{r} - \vec{r}')}$ . The implicit solution of the Schrödinger equation is given by  $\psi(\vec{r}) = \varphi(\vec{r}) + \int d^3r' G_+(\vec{r}, \vec{r}') U(\vec{r}') \psi(\vec{r}')$ , where  $\varphi(\vec{r})$  is a solution of the homogeneous Helmholtz equation (usually one takes  $\varphi(\vec{r}) = e^{ikz}$ , which is a general solution of the homogeneous equation with free parameters fixed by initial conditions). As a final step the implicit equation is solved iteratively.

³⁷An inverse operator is, so to speak, a generalisation of the Green function. Indeed, the inverse operator is defined by  $AA^{-1} = \mathbb{1}$ , the Green function by  $AG(\vec{r} - \vec{r}') = \delta(\vec{r} - \vec{r}')$  and the delta-function can be understood as a matrix-like representation of the unit operator  $\mathbb{1}$ .

It is quite straightforward to find the operator  $(E - H_0 + i\epsilon)^{-1}$ . One just has to realize that in the basis  $|\varphi_l\rangle$  in which the operator  $H_0$  is diagonal, one has  $E - H_0 + i\epsilon = \sum_l (E - \mathcal{E}_l + i\epsilon) |\varphi_l\rangle \langle \varphi_l|$ , where the sum, of course, stands for integrals over the continuous label  $l$ . As a direct consequence  $(E - H_0 + i\epsilon)^{-1} = \sum_l \frac{|\varphi_l\rangle \langle \varphi_l|}{E - \mathcal{E}_l + i\epsilon}$  and therefore

$$|\psi\rangle = |\varphi\rangle + \sum_l \frac{|\varphi_l\rangle \langle \varphi_l|}{E - \mathcal{E}_l + i\epsilon} \alpha H' |\psi\rangle$$

This implicit relation is solved iteratively, leading to the same structure as in the previous remark (matrix elements of  $H'$  in the numerator, energy differences in the denominator). The diagrams are as natural and useful as in the previous case.

As the last point let us focus not on the continuous, but rather on the discrete part of the spectrum. The analogue of the Lippmann-Schwinger equation becomes (in the  $\epsilon \rightarrow 0$  limit)

$$|\psi_n\rangle = |\varphi_n\rangle + \sum_{m \neq n} \frac{|\varphi_m\rangle \langle \varphi_m|}{E_n - \mathcal{E}_m} \alpha H' |\psi_n\rangle$$

This is now solved iteratively, leading to

$$|\psi_n\rangle = |\varphi_n\rangle + \alpha \sum_{m \neq n} \frac{|\varphi_m\rangle \langle \varphi_m| H' |\varphi_n\rangle}{E_n - \mathcal{E}_m} + \alpha^2 \sum_{m \neq n} \sum_{m' \neq n} \frac{|\varphi_m\rangle \langle \varphi_m| H' |\varphi_{m'}\rangle \langle \varphi_{m'}| H' |\varphi_n\rangle}{(E_n - \mathcal{E}_m)(E_n - \mathcal{E}_{m'})} + \text{higher terms}$$

where the higher terms have the same structure as the explicitly presented ones (note that the iterative solution provided the result in the form of power expansion in the parameter  $\alpha$ ). The final step is to multiply the iterative solution by  $\langle \varphi_n| H$  and to use  $\langle \varphi_n| H |\psi_n\rangle = E_n \langle \varphi_n| \psi_n\rangle$  and  $\langle \varphi_n| H |\varphi_n\rangle = \mathcal{E}_n \langle \varphi_n| \varphi_n\rangle + \alpha \langle \varphi_n| H' |\varphi_n\rangle$ . With the standard normalization (the same as in the Rayleigh-Schrödinger perturbation theory), i.e. for  $\langle \varphi_n| \varphi_n\rangle = \langle \varphi_n| \psi_n\rangle = 1$  one obtains the Brillouin-Wigner expansion

$$\begin{aligned} E_n = & \mathcal{E}_n + \alpha \langle \varphi_n| H' |\varphi_n\rangle + \alpha^2 \sum_{m \neq n} \frac{\langle \varphi_n| H' |\varphi_m\rangle \langle \varphi_m| H' |\varphi_n\rangle}{E_n - \mathcal{E}_m} \\ & + \alpha^3 \sum_{m \neq n} \sum_{m' \neq n} \frac{\langle \varphi_n| H' |\varphi_m\rangle \langle \varphi_m| H' |\varphi_{m'}\rangle \langle \varphi_{m'}| H' |\varphi_n\rangle}{(E_n - \mathcal{E}_m)(E_n - \mathcal{E}_{m'})} + \text{higher terms} \end{aligned}$$

**Remark:** As already mentioned in a footnote, the Feynman diagrams and rules presented here are different from the ones presented in the previous section (Conclusions). The reason is that they refer to different versions of the perturbation theory. A typical feature of the version discussed here (which is called the old-fashioned perturbation theory) is the presence of energy denominators (i.e. energy differences in denominators). The version presented in the Conclusions, on the other hand, did not contain such a structure in denominators, but rather something like  $p^2 - m^2 + i\epsilon$ . To get the version of Feynman diagrams and rules with these factors (which is much better suited for relativistic quantum theory), one should work with the time-dependent perturbation theory, not with the time-independent one. We will derive the Feynman rules for this version later on (see Chapter 2), in the framework of the relativistic quantum theory.

**Remark:** In the time-dependent perturbation theory the crucial object is the evolution operator  $U = e^{-iHt/\hbar}$ . In the quantum statistical physics the crucial object is the canonical density matrix  $\rho = e^{-\beta H}$ , where  $\beta = 1/kT$ . These two objects are closely related (by simple formal replacement  $it/\hbar \leftrightarrow \beta$ ) and one can therefore encounter the Feynman diagrams also in the statistical physics.

### 1.2.4 Quantum particles and classical fields

There is yet another important feature of the creation and annihilation operators, namely their classical limit which differs significantly from the notorious classical limit provided by the original Ehrenfest theorems. In their simplest one-dimensional version these theorems state that the expectation values of particle position and momentum operators satisfy quasi-classical equations

$$\frac{d\bar{p}}{dt} = -\overline{V'(x)} \quad \frac{d\bar{x}}{dt} = \frac{\bar{p}}{m}$$

where  $\bar{A} = \langle \psi | A | \psi \rangle$  for some state  $|\psi\rangle$  (not denoted explicitly, to avoid overloaded notation). The first equation is almost but not quite classical. It would be the classical Newton equation if its right-hand side was the value of the function  $V'$  at the mean position  $\bar{x}$ , rather than the mean value of this function. It therefore useful to write the Ehrenfest equations in this form

$$\frac{d\bar{p}}{dt} = -V'(\bar{x}) + \dots \quad \frac{d\bar{x}}{dt} = \frac{\bar{p}}{m}$$

where the ellipsis stand for the difference  $V'(\bar{x}) - \overline{V'(x)}$ . If this difference vanishes (as it does e.g. for the quadratic potential, i.e. for the linear derivative  $V'(x)$ ), the Ehrenfest equations for the expectation values are truly classical. If the difference is small, the equations are quasi-classical.³⁸

Now let us investigate the equations for the expectation values of the creation and annihilation operators. The general equation for the time evolution of the expectation value of any operator in any state (the Ehrenfest equations are just special cases of this equation) is well-known³⁹

$$i\hbar \frac{d}{dt} \bar{A} = \overline{[A, H]}$$

The commutators of the creation and annihilation operators with the simplest Hamiltonian of an ideal gas of free bosons

$$H = \int d^3k \, \varepsilon(\vec{k}) \, a_{\vec{k}}^+ a_{\vec{k}}$$

are easily calculated⁴⁰  $[a_{\vec{p}}^+, H] = -\varepsilon(\vec{p}) \, a_{\vec{p}}^+$   $[a_{\vec{p}}, H] = \varepsilon(\vec{p}) \, a_{\vec{p}}$  leading to

$$i\hbar \frac{d}{dt} \bar{a}_{\vec{p}}^+ = -\varepsilon(\vec{p}) \, \bar{a}_{\vec{p}}^+ \quad i\hbar \frac{d}{dt} \bar{a}_{\vec{p}} = \varepsilon(\vec{p}) \, \bar{a}_{\vec{p}}$$

These equations are exact ones – since the commutators are linear functions of the creation and annihilation operators, there are no ellipsis in the Ehrenfest-like equations for the free particles.

³⁸Let us emphasize that classical (or quasi-classical) equations for expectation values are not sufficient condition for the classical description of a system. Another important condition to be met is this: the expectation values must completely characterize the state of the system. This requires two things. First, typical expectation values are to be much greater than typical quantum uncertainties. And second, measurements precision should not reach the quantum uncertainties. This will play an important role in our discussion of the classical limit for the expectation values of the creation and annihilation operators.

³⁹The proof is straightforward. In the Schrödinger picture the equations follows from the fact that operators are time independent and states evolve according to the Schrödinger equation  $i\hbar \frac{d}{dt} |\psi(t)\rangle = H |\psi(t)\rangle$  and  $-i\hbar \frac{d}{dt} \langle \psi(t)| = \langle \psi(t)| H$  for the ket- and the bra-vectors respectively. The same result is, of course, obtained in the Heisenberg picture, where states are time independent and operators evolve according to the Heisenberg equation  $i\hbar \frac{\partial}{\partial t} A(t) = [A(t), H]$ .

⁴⁰ $[B, CD] = [B, C]D + C[B, D]$  and  $[a_{\vec{p}}, a_{\vec{k}}] = [a_{\vec{p}}^+, a_{\vec{k}}^+] = 0$ ,  $[a_{\vec{p}}, a_{\vec{k}}^+] = \delta(\vec{p} - \vec{k})$ .

What is the physical meaning of the equations for  $\bar{a}_{\vec{p}}^+$  and  $\bar{a}_{\vec{p}}$ ? These operators and their expectation values depend on the continuous variable  $\vec{p}$ . In classical physics quantities depending on the continuous variable  $\vec{x}$  are called fields. To see if  $\bar{a}_{\vec{p}}$  and  $\bar{a}_{\vec{p}}^+$  correspond to some familiar classical fields, let us re-write the equations in the  $x$ -representation.⁴¹ These relations, just like the Fourier transformation, convert derivatives to multiplications by the corresponding variable and vice versa. This conversion reads  $\vec{p} \leftrightarrow i\hbar\nabla$  for the creation operators and  $\vec{p} \leftrightarrow -i\hbar\nabla$  for the annihilation ones.⁴² The equations for⁴³  $\bar{a}^+(\vec{x}, t)$  and  $\bar{a}(\vec{x}, t)$  are therefore partial differential equations

$$i\hbar \frac{d}{dt} \bar{a}^+(\vec{x}, t) = -\varepsilon(i\hbar\nabla) \bar{a}^+(\vec{x}, t) \quad i\hbar \frac{d}{dt} \bar{a}(\vec{x}, t) = \varepsilon(-i\hbar\nabla) \bar{a}(\vec{x}, t)$$

Do these equations correspond to something familiar from the classical physics? Can one observe their manifestation at the classical level?

For non-relativistic bosonic particles with  $\varepsilon(\vec{p}) = \vec{p}^2/2m$  the equations become

$$i\hbar \frac{d}{dt} \bar{a}^+(\vec{x}, t) = \frac{\hbar^2}{2m} \Delta \bar{a}^+(\vec{x}, t) \quad i\hbar \frac{d}{dt} \bar{a}(\vec{x}, t) = -\frac{\hbar^2}{2m} \Delta \bar{a}(\vec{x}, t)$$

which is extremely well known, although not within classical physics – it's the Schrödinger equation for  $\bar{a}(\vec{x}, t)$  and complex conjugate equation for  $\bar{a}^+(\vec{x}, t)$ . How come that the trademark equation of quantum physics emerged naturally as a classical equation? And since it does, why there is no trace of it in the classical physics?

For relativistic bosonic particles with  $\varepsilon(\vec{p}) = \sqrt{\vec{p}^2 c^2 + m^2 c^4}$  the equations become

$$i\hbar \frac{d}{dt} \bar{a}^+(\vec{x}, t) = -\sqrt{m^2 c^4 - \hbar^2 c^2 \Delta} \bar{a}^+(\vec{x}, t) \quad i\hbar \frac{d}{dt} \bar{a}(\vec{x}, t) = \sqrt{m^2 c^4 - \hbar^2 c^2 \Delta} \bar{a}(\vec{x}, t)$$

what perhaps does not ring a bell. It is a common habit to get rid of the square root in these equations by taking time-derivative of both sides of the equations, leading to⁴⁴

$$\Delta \bar{a}^+(\vec{x}, t) - \frac{1}{c^2} \frac{d^2}{dt^2} \bar{a}^+(\vec{x}, t) = \frac{m^2 c^2}{\hbar^2} \bar{a}^+(\vec{x}, t) \quad \Delta \bar{a}(\vec{x}, t) - \frac{1}{c^2} \frac{d^2}{dt^2} \bar{a}(\vec{x}, t) = \frac{m^2 c^2}{\hbar^2} \bar{a}(\vec{x}, t)$$

which is quite well-known, but again not within the classical physics – it is the so-called Klein-Gordon equation, sometimes referred to as the relativistic Schrödinger equation (see the mostly historical remarks on the next page). Its appearance at the classical level is as mysterious as was the classical Schrödinger equation in the non-relativistic case. Only for massless particles one obtains something classically familiar – the Klein-Gordon equation for  $m = 0$  is nothing but the good old wave equation.

⁴¹The relations between the  $x$ - and  $p$ -representations for the creation and annihilation operators are (see page 26)  $a_{\vec{x}}^+ = \int \frac{d^3 p}{(2\pi\hbar)^{3/2}} e^{-i\vec{p}\cdot\vec{x}/\hbar} a_{\vec{p}}^+$  and  $a_{\vec{x}} = \int \frac{d^3 p}{(2\pi\hbar)^{3/2}} e^{i\vec{p}\cdot\vec{x}/\hbar} a_{\vec{p}}$ . Note that they correspond almost, but not quite, to the Fourier transformation. The reason for "almost" is the different sign in the exponents  $e^{\pm i\vec{p}\cdot\vec{x}/\hbar}$  for  $a^+$  and  $a$ .

⁴²Indeed  $i\hbar\nabla \bar{a}_{\vec{x}}^+ = \int \frac{d^3 p}{(2\pi\hbar)^{3/2}} i\hbar\nabla e^{-i\vec{p}\cdot\vec{x}/\hbar} \bar{a}_{\vec{p}}^+ = \int \frac{d^3 p}{(2\pi\hbar)^{3/2}} \vec{p} e^{-i\vec{p}\cdot\vec{x}/\hbar} \bar{a}_{\vec{p}}^+$  and this can be easily generalized to  $f(i\hbar\nabla) \bar{a}_{\vec{x}}^+ = \int \frac{d^3 p}{(2\pi\hbar)^{3/2}} f(\vec{p}) e^{-i\vec{p}\cdot\vec{x}/\hbar} \bar{a}_{\vec{p}}^+$  for any polynomial or Taylor expanded function  $f$ . For annihilation operators one gets in the same way  $f(-i\hbar\nabla) \bar{a}_{\vec{x}} = \int \frac{d^3 p}{(2\pi\hbar)^{3/2}} f(\vec{p}) e^{i\vec{p}\cdot\vec{x}/\hbar} \bar{a}_{\vec{p}}$ .

⁴³Sometimes (e.g. now) it is quite convenient to write the position  $\vec{x}$  as the variable rather than the index.

⁴⁴Let's write it down, even if it is rather trivial:

$\left(i\hbar \frac{d}{dt}\right)^2 \bar{a}^+(\vec{x}, t) = -i\hbar \frac{d}{dt} \sqrt{m^2 c^4 - \hbar^2 c^2 \Delta} \bar{a}^+(\vec{x}, t) = -\sqrt{m^2 c^4 - \hbar^2 c^2 \Delta} i\hbar \frac{d}{dt} \bar{a}^+(\vec{x}, t) = (m^2 c^4 - \hbar^2 c^2 \Delta) \bar{a}^+(\vec{x}, t)$

**Remark:** The Schrödinger equation  $i\hbar\partial_t\psi(\vec{x},t) = \left(\frac{\hbar^2}{2m}\Delta + U(\vec{x})\right)\psi(\vec{x},t)$  can be understood as the relation  $E = \frac{\vec{p}^2}{2m} + U(\vec{x})$  between the operators of energy  $\hat{H} = i\hbar\partial_t$  and momentum  $\hat{p}_i = -i\hbar\partial_i$ . If one starts from the relativistic relation  $E^2 = \vec{p}^2c^2 + m^2c^4$ , the so-called free Klein-Gordon equation is obtained in the similar way. It is a common habit to write this equation in the explicitly covariant form as  $\partial_\mu\partial^\mu\psi(\vec{x},t) = \frac{m^2c^2}{\hbar^2}\psi(\vec{x},t)$ . For sake of next remarks, let us note that it is not that straightforward to incorporate an interaction with an external field into the relativistic equation. One cannot introduce it directly via the potential energy, since this notion does not make much sense in a relativistic theory (action at distance vs. relativity of simultaneity for nonlocal events). One can, however, obtain a relativistic equation for interaction with an external electromagnetic field by the standard replacement of 4-momentum  $p_\mu \rightarrow p_\mu + qA_\mu$  (precisely this transformation is in fact used in the standard quantum mechanics to obtain the Pauli equation from the Schrödinger equation). The Klein-Gordon equation for the quantum particle in the classical electromagnetic field is therefore  $(i\hbar\partial_\mu - qA_\mu)(i\hbar\partial^\mu - qA^\mu)\psi(\vec{x},t) = m^2c^2\psi(\vec{x},t)$ . For vanishing 3-vector potential and time independent scalar potential this equation looks (in a given reference frame) like a relativistic equation with potential energy (e. g. the Coulomb one).

**Remark:** The first physicist ever to use the Klein-Gordon equation was Schrödinger himself. He solved the relativistic equation for the hydrogen atom even before his non-relativistic equation. The reason why he did not publish this solution is quite interesting. The spectrum of the hydrogen atom came out non-degenerate from the relativistic equation. This was OK, since the spectrum is indeed non-degenerate – the splitting of energy levels is known as "the fine structure". On the other hand, it was far from being OK, because the splitting was not consistent with the experimental data. (The reason was, as we know today, that the Klein-Gordon equation does not take into account the spin of the electron, which is also relevant for the fine splitting. The relativistic equation for the particle with spin  $\frac{1}{2}$  discovered later by Dirac gives the correct fine splitting for the hydrogen spectrum.) Only after his failure to get correct fine splitting Schrödinger turned his attention to the non-relativistic equation and published the results. He obviously considered no splitting to be preferable to the wrong splitting.

**Remark:** The function  $\psi$  in the Schrödinger equation enjoys the simple probabilistic interpretation, but for the Klein-Gordon equation this is not true anymore. Let us recall that in former case the overall probability is conserved due to the continuity equation  $\partial_t|\psi|^2 + \text{div}\vec{j} = 0$  where  $\vec{j} = \frac{i\hbar}{2m}(\psi\nabla\psi^* - \psi^*\nabla\psi)$ . One can obtain a similar equation (along the same lines) for the Klein-Gordon equation, the result is  $\partial_\mu j^\mu = 0$  where  $j^\mu = \psi^*\partial^\mu\psi - \psi\partial^\mu\psi^*$ . The component  $j^0$ , however, can be negative, so it cannot be interpreted as a probability density. The connection between the Schrödinger and Klein-Gordon equations is not as straightforward as one might expect.

**Remark:** The linear Klein-Gordon equation based on the relation  $E^2 = \vec{p}^2c^2 + m^2c^4$  is clearly much more pleasant to deal with than the non-linear equation obtained from  $E = \sqrt{\vec{p}^2c^2 + m^2c^4}$ . Nicer equation, however, has its price – namely the negative kinetic energy solutions of the quadratic equation. Solutions corresponding to such energies plague the Klein-Gordon equation in a non-trivial way. For the free Klein-Gordon equation this does not represent a serious problem (if one starts in the positive energy subspace, the time evolution does not lead out of this subspace). Once the interaction with the external classical electromagnetic field is switched on, the problem becomes a serious one (the time evolution leads the solution outside the positive energy subspace).

**Remark:** We are not going to discuss the above mentioned difficulties (negative probabilities, negative kinetic energies) of the Klein-Gordon equation understood as a relativistic Schrödinger equation here. For us it emerged as a quasi-classical equation for an expectation value of the creation and annihilation operators, not as a quantum equation for the wave-function.

What kind of classical waves do the fields  $\bar{a}^+(\vec{x}, t)$  and  $\bar{a}(\vec{x}, t)$  for massless particles correspond to? Due to the presence of the speed of light, the equations look almost, but not quite, like the equations for free electromagnetic fields or potentials. The difference is twofold. First, the electromagnetic fields or potentials are real quantities, while expectation values of the creation and annihilation operators are complex (since the creation and annihilation operators are not hermitian). Second, electromagnetic fields and potentials are 3-vectors and 4-vector respectively, while  $\bar{a}^+(\vec{x}, t)$  and  $\bar{a}(\vec{x}, t)$  are neither vectors, nor their components. Nevertheless, the case of massless particles seems to be quite promising and definitely worth further investigation.

Complex physical quantities can be encountered also in classical physics, but usually only as auxiliary ones. So if one wants to obtain equations for some basic classical quantities, it is perhaps reasonable to study not the creation and annihilation operators themselves, but rather some hermitian operators constructed thereof. The most natural option seems to be the sum and  $i$  times the difference of  $a_{\vec{x}}^+$  and  $a_{\vec{x}}$ . So let us define

$$\Phi_{\vec{x}} = a_{\vec{x}}^+ + a_{\vec{x}} \quad \Pi_{\vec{x}} = i(a_{\vec{x}}^+ - a_{\vec{x}})$$

Now, since in both non-relativistic and relativistic cases  $\varepsilon(\vec{p}) = \varepsilon(-\vec{p})$ , the Ehrenfest-like equations for  $\bar{a}^+(\vec{x}, t)$  and  $\bar{a}(\vec{x}, t)$  can be immediately rewritten as equations for  $\bar{\Phi}(\vec{x}, t)$  and  $\bar{\Pi}(\vec{x}, t)$

$$\hbar \frac{d}{dt} \bar{\Phi}(\vec{x}, t) = \varepsilon(i\hbar\nabla) \bar{\Pi}(\vec{x}, t) \quad \hbar \frac{d}{dt} \bar{\Pi}(\vec{x}, t) = -\varepsilon(i\hbar\nabla) \bar{\Phi}(\vec{x}, t)$$

Combining these two equations one obtains

$$\hbar^2 \frac{d^2}{dt^2} \bar{\Phi}(\vec{x}, t) = -\varepsilon^2(i\hbar\nabla) \bar{\Phi}(\vec{x}, t) \quad \hbar^2 \frac{d^2}{dt^2} \bar{\Pi}(\vec{x}, t) = -\varepsilon^2(i\hbar\nabla) \bar{\Pi}(\vec{x}, t)$$

which for the relativistic particles are just the Klein-Gordon equations and for massless particles they become the wave equations, now for the real fields  $\bar{\Phi}(\vec{x}, t)$  and  $\bar{\Pi}(\vec{x}, t)$ .

One can try to push the analogy with electromagnetic fields even further and find out, whether some quantum interaction of our massless particles with some massive particles lead to something similar to classical electromagnetism. As the most simple possibility let us investigate a theory of massless particles interacting with some non-relativistic particles. The form of the interaction can be guessed from analogy with photons.

We know that charged particles (e. g. electrons in atoms) can emit or absorb photons. Let us assume something similar in our case. A transition of the massive particle from a state  $|k\rangle$  to a state  $|j\rangle$  with simultaneous emission of the massless particle should be described by an interaction hamiltonian of the form  $a_i^+ b_j^+ b_k$ , where  $a^+$ ,  $a$  and  $b^+$ ,  $b$  are the creation and annihilation operators of the massless and massive particles respectively. If the interaction is local, then the interaction hamiltonian becomes

$$H_{\text{int}} = \int d^3x \, g a_{\vec{x}}^+ b_{\vec{x}}^+ b_{\vec{x}} + \text{h.c.} = \int d^3x \, g (a_{\vec{x}}^+ + a_{\vec{x}}) b_{\vec{x}}^+ b_{\vec{x}} = \int d^3x \, g \Phi_{\vec{x}} b_{\vec{x}}^+ b_{\vec{x}}$$

and the full hamiltonian is therefore

$$H = H_0 + H_{\text{int}} = \int d^3k \, \varepsilon(\vec{k}) a_{\vec{k}}^+ a_{\vec{k}} + \int d^3p \, E(\vec{p}) b_{\vec{p}}^+ b_{\vec{p}} + \int d^3x \, g \Phi_{\vec{x}} b_{\vec{x}}^+ b_{\vec{x}}$$

where  $\varepsilon(\vec{k}) = kc$  and  $E(\vec{p}) = \vec{p}^2/2m$ . We are now interested in Ehrenfest-like equations for the operator  $\Phi_{\vec{x}}$  as well as for the center of mass position  $\vec{X}$  and the total momentum  $\vec{P}$  of the system of massive particles. Do they look like something similar to the classical electrodynamics?

The operators  $\vec{X}$  and  $\vec{P}$  can be readily written in terms of  $b^+$  and  $b$  operators as

$$\vec{X} = \frac{1}{M} \int d^3x \vec{x} m b_{\vec{x}}^+ b_{\vec{x}} \quad \vec{P} = \int d^3p \vec{p} b_{\vec{p}}^+ b_{\vec{p}}$$

where  $m b_{\vec{x}}^+ b_{\vec{x}}$  is the mass density operator and  $M = \langle \psi | \int d^3x m b_{\vec{x}}^+ b_{\vec{x}} | \psi \rangle$  is the total mass of the system. For the free system the Ehrenfest theorems for  $\vec{X}$  and  $\vec{P}$  are⁴⁵ the expected ones:  $\frac{d}{dt} \vec{X} = \frac{1}{M} \vec{P}$  and  $\frac{d}{dt} \vec{P} = 0$ . For the system with interaction they are⁴⁶

$$\frac{d}{dt} \vec{X} = \frac{1}{M} \vec{P} \quad \frac{d}{dt} \vec{P} = -g \int d^3x \overline{b_{\vec{x}}^+ b_{\vec{x}}} \nabla \Phi_{\vec{x}}$$

If the state  $|\psi\rangle$  in the definition of the expectation value is a direct product of a state of massive particles and a state of massless particelles, i. e. if  $|\psi\rangle = |\psi_A\rangle |\psi_B\rangle$ , then  $\overline{b_{\vec{x}}^+ b_{\vec{x}}} \nabla \Phi_{\vec{x}} = \overline{b_{\vec{x}}^+ b_{\vec{x}}} \nabla \Phi_{\vec{x}}$  and the Ehrenfest theorem for  $\vec{P}$  becomes an old friend: the time derivative of the momentum is equal to the force which is given by the integral of the "charge" density  $g \overline{b_{\vec{x}}^+ b_{\vec{x}}}$  multiplied by the minus gradient of the "potential"  $\Phi_{\vec{x}}$ .

To find out how the interaction modifies the Ehrenfest equation for  $\bar{\Phi}(\vec{x}, t)$  and  $\bar{\Pi}(\vec{x}, t)$  one has to calculate commutators of  $\Phi_{\vec{x}}$  and  $\Pi_{\vec{y}}$  with the interaction hamiltonian. This is straightforward, using  $[\Phi_{\vec{x}}, \Phi_{\vec{y}}] = [\Pi_{\vec{x}}, \Pi_{\vec{y}}] = 0$  and  $[\Phi_{\vec{x}}, \Pi_{\vec{y}}] = 2i\delta^3(\vec{x} - \vec{y})$  (check it), the result is

$$\hbar \frac{d}{dt} \bar{\Phi}(\vec{x}, t) = \varepsilon(i\hbar \nabla) \bar{\Pi}(\vec{x}, t) \quad \hbar \frac{d}{dt} \bar{\Pi}(\vec{x}, t) = -\varepsilon(i\hbar \nabla) \bar{\Phi}(\vec{x}, t) - 2g \overline{b_{\vec{x}}^+ b_{\vec{x}}}$$

leading to the wave equations with the source term  $\frac{2g}{\hbar^2} \varepsilon(i\hbar \nabla) \overline{b_{\vec{x}}^+ b_{\vec{x}}}$  (check it). If we wanted to interpret  $\bar{\Phi}(\vec{x}, t)$  as a classical potential, we would rather expect the "charge" density  $g \overline{b_{\vec{x}}^+ b_{\vec{x}}}$  as the source term. So at the very end our attempt to find a familiar classical limit has failed.

⁴⁵Both theorems are special cases of  $i\hbar \frac{d}{dt} \bar{A} = [\bar{A}, H]$  with  $A$  being either  $\vec{P}$  or  $\vec{X}$  and the free hamiltonian being  $\int d^3p E(\vec{p}) b_{\vec{p}}^+ b_{\vec{p}}$ . For commutators one uses  $[BC, DE] = B[C, D]E + [B, D]CE + DB[C, E] + D[B, E]C$ . This vanishes for  $\vec{P}$  (check it), while for  $\vec{X}$  one obtains  $[b_{\vec{x}}^+ b_{\vec{x}}, b_{\vec{p}}^+ b_{\vec{p}}] = \frac{e^{i\vec{p} \cdot \vec{x}/\hbar}}{(2\pi\hbar)^{3/2}} b_{\vec{x}}^+ b_{\vec{p}} - \frac{e^{-i\vec{p} \cdot \vec{x}/\hbar}}{(2\pi\hbar)^{3/2}} b_{\vec{p}}^+ b_{\vec{x}}$  (check it). Now comes a tricky part. The commutator

$$[\vec{X}, H] = \frac{m}{M} \int d^3x d^3p \vec{x} E(\vec{p}) [b_{\vec{x}}^+ b_{\vec{x}}, b_{\vec{p}}^+ b_{\vec{p}}] = \frac{m}{M} \int \frac{d^3x d^3p}{(2\pi\hbar)^{3/2}} \vec{x} E(\vec{p}) \left( e^{i\vec{p} \cdot \vec{x}/\hbar} b_{\vec{x}}^+ b_{\vec{p}} - e^{-i\vec{p} \cdot \vec{x}/\hbar} b_{\vec{p}}^+ b_{\vec{x}} \right)$$

is rewritten in terms of  $b_{\vec{y}}^+$  and  $b_{\vec{y}}$  operators and in the second integral the variables are interchanged ( $\vec{x} \leftrightarrow \vec{y}$ )

$$\begin{aligned} \frac{m}{M} \int \frac{d^3x d^3y d^3p}{(2\pi\hbar)^3} \vec{x} E(\vec{p}) \left( e^{i\vec{p} \cdot (\vec{x}-\vec{y})/\hbar} b_{\vec{x}}^+ b_{\vec{y}} - e^{-i\vec{p} \cdot (\vec{x}-\vec{y})/\hbar} b_{\vec{y}}^+ b_{\vec{x}} \right) = \\ \frac{m}{M} \int \frac{d^3x d^3y d^3p}{(2\pi\hbar)^3} (\vec{x} - \vec{y}) E(\vec{p}) e^{i\vec{p} \cdot (\vec{x}-\vec{y})/\hbar} b_{\vec{x}}^+ b_{\vec{y}} = \frac{m}{M} \int \frac{d^3x d^3y d^3p}{(2\pi\hbar)^3} b_{\vec{x}}^+ b_{\vec{y}} E(\vec{p}) (-i\hbar \nabla_{\vec{p}}) e^{i\vec{p} \cdot (\vec{x}-\vec{y})/\hbar} \end{aligned}$$

and the partial integration finally leads to

$$[\vec{X}, H_0] = \frac{m}{M} \int \frac{d^3x d^3y d^3p}{(2\pi\hbar)^3} b_{\vec{x}}^+ b_{\vec{y}} (i\hbar \nabla_{\vec{p}} E(\vec{p})) e^{i\vec{p} \cdot (\vec{x}-\vec{y})/\hbar} = \frac{i\hbar}{M} \int d^3p \vec{p} b_{\vec{p}}^+ b_{\vec{p}} = \frac{i\hbar}{M} \vec{P}$$

⁴⁶The commutator of  $\vec{X}$  with the interaction hamiltonian vanishes (check it). For the commutator of  $\vec{P}$  with the interaction hamiltonian one uses basically the same tricks as in the previous footnote to get

$$\begin{aligned} [\vec{P}, H_{\text{int}}] &= g \int d^3p d^3x \vec{p} [b_{\vec{p}}^+ b_{\vec{p}}, b_{\vec{x}}^+ b_{\vec{x}}] \Phi_{\vec{x}} = g \int \frac{d^3p d^3q d^3x}{(2\pi\hbar)^3} (\vec{p} - \vec{q}) e^{-i(\vec{p}-\vec{q}) \cdot \vec{x}/\hbar} b_{\vec{p}}^+ b_{\vec{q}} \Phi_{\vec{x}} \\ &= g \int \frac{d^3p d^3q d^3x}{(2\pi\hbar)^3} b_{\vec{p}}^+ b_{\vec{q}} \Phi_{\vec{x}} i\hbar \nabla e^{-i(\vec{p}-\vec{q}) \cdot \vec{x}/\hbar} = -i\hbar g \int d^3x b_{\vec{x}}^+ b_{\vec{x}} \nabla \Phi_{\vec{x}} \end{aligned}$$

### a toy model of electrodynamics

There is, fortunately, a simple way to modify the operators  $\Phi_{\vec{x}}$  and  $\Pi_{\vec{x}}$  in such a way that the resulting classical limit turns out to be completely analogous to the classical electrodynamics. Let us summarize what we have done so far. Starting from the equations of motion for  $\bar{a}_{\vec{p}}^+$  and  $\bar{a}_{\vec{p}}$  we have derived the equations of motion for their specific linear combinations  $\bar{\Phi}(\vec{x}, t)$  and  $\bar{\Pi}(\vec{x}, t)$ . These equations contained one trouble-maker term, namely the  $\varepsilon(i\hbar\nabla)$  term in the equation for  $\frac{d}{dt}\bar{\Phi}(\vec{x}, t)$ . It was just this term that spoiled the decent "charge" density source term  $g\bar{b}_{\vec{x}}^+b_{\vec{x}}$  in the wave equation for  $\Phi_{\vec{x}}$  (this is important and the reader should see it clearly).

One can repeat the whole procedure with slightly more general hermitian linear combinations

$$\begin{aligned}\varphi_{\vec{x}} &= \int \frac{d^3p}{(2\pi\hbar)^{3/2}} c_{\vec{p}} \left( e^{-i\vec{p}\cdot\vec{x}/\hbar} a_{\vec{p}}^+ + e^{i\vec{p}\cdot\vec{x}/\hbar} a_{\vec{p}} \right) \\ \pi_{\vec{x}} &= \int \frac{d^3p}{(2\pi\hbar)^{3/2}} c'_{\vec{p}} i \left( e^{-i\vec{p}\cdot\vec{x}/\hbar} a_{\vec{p}}^+ - e^{i\vec{p}\cdot\vec{x}/\hbar} a_{\vec{p}} \right)\end{aligned}$$

where  $c_{\vec{p}}$  and  $c'_{\vec{p}}$  are some real coefficients.⁴⁷ With a proper choice of these coefficients one can get rid of the trouble-maker term. Indeed, the Ehrenfest-like equations for these operators in case of free particles are

$$\begin{aligned}\hbar \frac{d}{dt} \bar{\varphi}(\vec{x}, t) &= \int \frac{d^3p}{(2\pi\hbar)^{3/2}} c_{\vec{p}} \varepsilon(\vec{p}) i \left( e^{-i\vec{p}\cdot\vec{x}/\hbar} \bar{a}_{\vec{p}}^+ - e^{i\vec{p}\cdot\vec{x}/\hbar} \bar{a}_{\vec{p}} \right) \\ \hbar \frac{d}{dt} \bar{\pi}(\vec{x}, t) &= \int \frac{d^3p}{(2\pi\hbar)^{3/2}} c'_{\vec{p}} \varepsilon(\vec{p}) \left( e^{-i\vec{p}\cdot\vec{x}/\hbar} \bar{a}_{\vec{p}}^+ + e^{i\vec{p}\cdot\vec{x}/\hbar} \bar{a}_{\vec{p}} \right)\end{aligned}$$

and for the specific choice

$$c_{\vec{p}} \varepsilon(\vec{p}) = \hbar c'_{\vec{p}}$$

one obtains

$$\frac{d}{dt} \bar{\varphi}(\vec{x}, t) = \bar{\pi}(\vec{x}, t) \quad \hbar^2 \frac{d}{dt} \bar{\pi}(\vec{x}, t) = -\varepsilon^2(i\hbar\nabla) \bar{\varphi}(\vec{x}, t)$$

as needed. For massless particles these two equations lead to

$$\frac{d^2}{dt^2} \bar{\varphi}(\vec{x}, t) - c^2 \Delta \bar{\varphi}(\vec{x}, t) = 0$$

which is the same wave equation as the one for  $\bar{\Phi}(\vec{x}, t)$  in case of free massless particles. How is this equation modified in the presence of interactions? Since the theory is now formulated in terms of  $\varphi_{\vec{x}}$  and  $\pi_{\vec{x}}$  rather than  $\Phi_{\vec{x}}$  and  $\Pi_{\vec{x}}$ , it is quite reasonable to investigate the modified interaction term obtained by the replacement  $\Phi_{\vec{x}} \rightarrow \varphi_{\vec{x}}$ , i. e.

$$H_{\text{int}} = \int d^3x g \varphi_{\vec{x}} b_{\vec{x}}^+ b_{\vec{x}}$$

The commutators of the operators  $\varphi_{\vec{x}}$  and  $\pi_{\vec{x}}$  with this interaction hamiltonian are

$$[\varphi_{\vec{x}}, H_{\text{int}}] = 0 \quad [\pi_{\vec{x}}, H_{\text{int}}] = \int d^3y g [\pi_{\vec{x}}, \varphi_{\vec{y}}] b_{\vec{y}}^+ b_{\vec{y}}$$

which means that the wave equation for  $\bar{\varphi}(\vec{x}, t)$  obtains a RHS equal to  $\frac{g}{i\hbar} \int d^3y [\pi_{\vec{x}}, \varphi_{\vec{y}}] \overline{b_{\vec{y}}^+ b_{\vec{y}}}$ .

⁴⁷For  $c_{\vec{p}} = c'_{\vec{p}} \equiv 1$  the new operators  $\varphi_{\vec{x}}$  and  $\pi_{\vec{x}}$  are just the old ones  $\Phi_{\vec{x}}$  and  $\Pi_{\vec{x}}$ , so the modification is a kind of generalization. Why is this particular generalization worth investigating? The fair answer is that it was introduced without any deep motivation, simply because it leads quickly to the desired result (this is a common excuse for artificial steps). It is not unnatural, especially if one recalls the notoriously known LHO relations  $\hat{x} = c(a + a^+)$  and  $\hat{p} = ic'(a - a^+)$  (with the specific choice of  $c$  and  $c'$ ), but this does not make them natural. So it may come as some relief that in the section about canonical dequantization and quantization the "generalized" operators  $\varphi_{\vec{x}}$  and  $\pi_{\vec{x}}$  will appear again in a more natural way.

Did we get what we were after? Did we get  $g \overline{b_x^+ b_x}$  (perhaps with the minus sign, as we shall discuss in a while) on the RHS of the wave equation? The answer is clearly affirmative, provided  $[\pi_{\vec{x}}, \varphi_{\vec{y}}] = \pm i \hbar \delta^3(\vec{x} - \vec{y})$ . So the next question is, whether one can find the coefficients  $c_{\vec{p}}$  and  $c'_{\vec{p}}$  ensuring this commutation relation. The answer is again affirmative – it is straightforward to check⁴⁸ that any functions satisfying

$$c_{\vec{p}} c'_{\vec{p}} = \mp \hbar / 2$$

would do the job. This is the second condition for the coefficients (the first one was  $c_{\vec{p}} \varepsilon(\vec{p}) = \hbar c'_{\vec{p}}$ ). These two conditions determine the coefficients unambiguously

$$c_{\vec{p}} = \frac{\hbar}{\sqrt{\mp 2 \varepsilon(\vec{p})}} \quad c'_{\vec{p}} = \sqrt{\frac{\mp \varepsilon(\vec{p})}{2}}$$

and these solutions are real only for the lower sign  $+$ . So finally we have reached the specific operator  $\varphi_{\vec{x}}$  for which the Ehrenfest theorems in our toy model lead to the wave equation with the standard source term⁴⁹

$$\frac{d^2}{dt^2} \bar{\varphi}(\vec{x}, t) - c^2 \Delta \bar{\varphi}(\vec{x}, t) = -g \overline{b_x^+ b_x}$$

As to the operators  $\vec{X}$  and  $\vec{P}$ , the only change in the equations for their expectation values is the replacement  $\Phi_{\vec{x}} \rightarrow \varphi_{\vec{x}}$ , so the Ehrenfest theorems for these two operators are the ones for the centre of mass and the total momentum of particles under the influence of the force  $-g \nabla \bar{\varphi}_{\vec{x}}$  (if we consider specific states  $|\psi\rangle = |\psi_A\rangle |\psi_B\rangle$ ).

Let us summarize: The simple model at the particle level

$$H = \int d^3 k \, k c \, a_k^+ a_k + \frac{1}{2m} \int d^3 p \, p^2 \, b_p^+ b_p + \int d^3 x \, g \, \varphi_{\vec{x}} b_x^+ b_x$$

where

$$\begin{aligned} \varphi_{\vec{x}} &= \int \frac{d^3 p}{(2\pi\hbar)^{3/2}} \frac{\hbar}{\sqrt{2\varepsilon(\vec{p})}} \left( e^{-i\vec{p}\cdot\vec{x}/\hbar} a_p^+ + e^{i\vec{p}\cdot\vec{x}/\hbar} a_{\vec{p}} \right) \\ \pi_{\vec{x}} &= \int \frac{d^3 p}{(2\pi\hbar)^{3/2}} \sqrt{\frac{\varepsilon(\vec{p})}{2}} i \left( e^{-i\vec{p}\cdot\vec{x}/\hbar} a_p^+ - e^{i\vec{p}\cdot\vec{x}/\hbar} a_{\vec{p}} \right) \end{aligned}$$

leads to a toy model of semi-relativistic classical electrodynamics⁵⁰

$$\begin{aligned} \frac{d}{dt} \vec{X} &= \frac{1}{M} \vec{P} & \frac{d}{dt} \vec{P} &= -g \int d^3 x \, \overline{b_x^+ b_x} \nabla \bar{\varphi}_{\vec{x}} \\ \frac{d}{dt} \bar{\varphi}(\vec{x}, t) &= \bar{\pi}(\vec{x}, t) & \frac{d}{dt} \bar{\pi}(\vec{x}, t) &= c^2 \Delta \bar{\varphi}(\vec{x}, t) - g \overline{b_x^+ b_x} \end{aligned}$$

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⁴⁸ $[\pi_{\vec{x}}, \varphi_{\vec{y}}] = \int \frac{d^3 p \, d^3 q}{(2\pi\hbar)^3} i c'_{\vec{p}} c_{\vec{q}} [e^{-i\vec{p}\cdot\vec{x}/\hbar} a_p^+ - e^{i\vec{p}\cdot\vec{x}/\hbar} a_{\vec{p}}, e^{-i\vec{q}\cdot\vec{y}/\hbar} a_q^+ + e^{i\vec{q}\cdot\vec{y}/\hbar} a_{\vec{q}}]$  and now one uses the commutation relations for the creation and annihilation operators to get  $[\pi_{\vec{x}}, \varphi_{\vec{y}}] = - \int \frac{d^3 p}{(2\pi\hbar)^3} i c_{\vec{p}} c'_{\vec{p}} (e^{-i\vec{p}\cdot(\vec{x}-\vec{y})/\hbar} + e^{i\vec{p}\cdot(\vec{x}-\vec{y})/\hbar})$ .

The final step uses  $\int \frac{d^3 x}{(2\pi)^3} e^{-i\vec{k}\cdot\vec{x}} = \delta^3(\vec{k})$  which means that if  $c_{\vec{p}} c'_{\vec{p}} = \text{const}$  then  $[\pi_{\vec{x}}, \varphi_{\vec{y}}] = -2i \text{const} \delta^3(\vec{x} - \vec{y})$ .

⁴⁹The term is standard, but the sign is not. In the classical electrodynamics the wave equation for the scalar potential in the Lorenz gauge reads  $\frac{1}{c^2} \frac{d^2}{dt^2} \varphi(\vec{x}, t) - \Delta \varphi(\vec{x}, t) = \frac{1}{\epsilon} \rho(\vec{x}, t)$ . In our wave equation for an expectation value  $\bar{\varphi}(\vec{x}, t)$  we have  $-g \overline{b_x^+ b_x}$  on the RHS, which is nothing but the "charge" density, but with the minus sign. For a discussion of an important physical consequence of this sign see the remarks the next page.

⁵⁰Let us note that the equation for  $\bar{\varphi}(\vec{x}, t)$  is the wave equation with the expected source term (up to the sign)

$$\frac{d^2}{dt^2} \bar{\varphi}(\vec{x}, t) - c^2 \Delta \bar{\varphi}(\vec{x}, t) = -g \overline{b_x^+ b_x}$$

**Remark:** Let us consider a heavy particle at the origin of the coordinate system. What classical field  $\bar{\varphi}(\vec{x}, t)$  does it generate in our toy model of electrodynamics? In the limit of infinite mass the momentum of the particle does not change within the classical approximation (any change would require infinite force). i. e. in the classical limit the source is stationary. For a stationary source one would expect a time independent field, so let us focus on stationary states  $|\psi\rangle = |\psi_A\rangle|\psi_B\rangle$  in the definition of the expectation value. In such case the time derivative in the equation for  $\bar{\varphi}(\vec{x})$  vanishes and we are left with the Poisson equation  $c^2 \Delta \bar{\varphi}(\vec{x}) = g \delta(\vec{x})$  since for  $|\psi_B\rangle = |\vec{x} = \vec{0}\rangle$  one obtains  $g b_{\vec{x}}^+ b_{\vec{x}} = g \delta(\vec{x})$ . The solution of this equation for proper boundary conditions (vanishing at infinity) is the notoriously known Coulomb-like potential

$$\bar{\varphi}(\vec{x}) = -\frac{g}{4\pi c^2} \frac{1}{|\vec{x}|}$$

**Remark:** Let us now consider yet another particle  $C$ , with the same "charge" and different mass, interacting with the massless particles in the same way as the heavy particle

$$H = \int d^3k \, k \, c \, a_{\vec{k}}^+ a_{\vec{k}} + \int d^3p \, \frac{\vec{p}^2}{2M} \, b_{\vec{p}}^+ b_{\vec{p}} + \int d^3p \, \frac{\vec{p}^2}{2m} \, c_{\vec{p}}^+ c_{\vec{p}} + \int d^3x \, g \, \varphi_{\vec{x}} (b_{\vec{x}}^+ b_{\vec{x}} + c_{\vec{x}}^+ c_{\vec{x}})$$

In the state with just one heavy and one light particle, the new particle generates a classical field  $\bar{\varphi}(\vec{x})$  of it's own, but this field influences neither the heavy particle (because of the infinite mass), nor the light one (because the particle cannot catch up with it's own field propagating with the speed of light). So in the classical limit this new particle feels only the Coulomb-like field of the heavy particle, i.e. we have obtained the Ehrenfest equation with the Coulomb-like force

$$\vec{F}(\vec{x}) = -\frac{g^2}{4\pi c^2} \frac{\vec{x}}{|\vec{x}|^3}$$

Our toy model has lead us to the Rutheford-like model of the hydrogen atom. Unlike the electrostatic force for equal charges, the force is attractive (due to the minus sign). This is a consequence of the "wrong" sign in the wave equation for the  $\bar{\varphi}(\vec{x}, t)$ .

**Remark:** If the light particle from the previous remark was really light and if it was close to the heavy particle, the classical limit would hardly provide a decent approximation. Nevertheless, the classical limit seems to be reasonable for the heavy particle and also for the massless particles "created by the heavy one". In the limit of infinitely heavy particle we therefore replace part of the operator  $\varphi(\vec{x}, t)$  by its expectation value, i.e. by the Coulomb-like potential  $-\frac{g}{4\pi c^2} \frac{1}{|\vec{x}|}$  and besides that, we won't consider the (infinitely) heavy particle. This leads to the effective Hamiltonian

$$H = \int d^3k \, k \, c \, a_{\vec{k}}^+ a_{\vec{k}} + \int d^3p \, \frac{\vec{p}^2}{2m} \, c_{\vec{p}}^+ c_{\vec{p}} - \int d^3x \, \frac{g}{4\pi c^2} \frac{1}{|\vec{x}|} c_{\vec{x}}^+ c_{\vec{x}} + \int d^3x \, g \, \varphi_{\vec{x}} c_{\vec{x}}^+ c_{\vec{x}}$$

The second and the third term correspond to the Hamiltonian of non-relativistic particles in the external Coulomb-like potential. For one light particle states this Hamiltonian leads to the Schrödinger equation for the hydrogen-like atom. The first and the last term in the Hamiltonian correspond to the spontaneous emission (and absorption) of massless photon-like particles. Our toy model has lead us to the improved Schrödinger-like model of the hydrogen atom.

**Remark:** If one considers a massive (with the mass  $\mu$ ) instead of massless particles interacting with the infinitely heavy particle, then the reasoning used in the first remark lead us to the equation  $c^2 \Delta \bar{\varphi}(\vec{x}) - \frac{\mu^2 c^2}{\hbar^2} \bar{\varphi}(\vec{x}) = g \delta(\vec{x})$  with the solution  $\bar{\varphi}(\vec{x}) = -\frac{g}{4\pi c^2} \frac{1}{|\vec{x}|} e^{-\mu c |\vec{x}|/\hbar}$ . This is a short-ranged potential with the range related to the mass of the particle. Our toy model with massive particles has lead us to the Yukawa potential and his model of nuclear interactions.

### canonical quantization

In the previous paragraph we have struggled quite a bit to find the specific linear combinations of the creation and annihilation operators leading to the particular classical limit inspired by the electromagnetism. And although it was instructive (at least according to the present author) this is not how the said linear combinations normally enter the game. They typically emerge via the procedure called canonical quantization, which we are going to discuss briefly now (and in much more detail later on).

The canonical quantization is based on the observation (first made by Dirac) of a remarkable connection between quantum and classical mechanics, namely between commutators and Poisson brackets. Thanks to this connection one can establish an important correspondence between the Heisenberg formulation of quantum mechanics and the Hamiltonian formulation of classical mechanics — the Ehrenfest equations in the former are simply the Hamilton equations of the latter. The link between the two theories (the quantum one and the classical one) is quite straightforward, so one can move between them fairly easily. If one wants to have a quantum theory with a given classical limit (as we did in the previous paragraph) then perhaps the best way to proceed is to formulate the classical theory in the Hamiltonian formalism with Poisson brackets and then use the said correspondence between the two to obtain the desired quantum theory.

Let us now demonstrate the "canonical" link between classical and quantum physics in the simplest case of point masses (without constraints⁵¹). Later on, we will need this link for classical field theory⁵² rather than for classical mechanics, and we will develop the required formalism in the second chapter. But to understand the main point, the simplest example is sufficient.

The Hamilton equations of classical mechanics are frequently formulated in terms of the Poisson brackets as

$$\frac{d}{dt}A(q, p) = \{A(q, p), H(q, p)\}$$

where the Poisson brackets are defined as  $\{B, C\} = \sum_i \frac{\partial B}{\partial q_i} \frac{\partial C}{\partial p_i} - \frac{\partial B}{\partial p_i} \frac{\partial C}{\partial q_i}$  (beware of different overall sign used by different authors). The brackets are usually evaluated by explicit differentiation. This, however, is not the only possibility. An alternative version of their evaluation is provided by two properties of the brackets which follow directly from the definition:

- $\{B, CD\} = \{B, C\}D + C\{B, D\} \quad \{BC, D\} = B\{C, D\} + \{B, D\}C$
- $\{q_i, q_j\} = \{p_i, p_j\} = 0 \quad \{q_i, p_j\} = \delta_{ij}$

If the functions  $A(q, p)$  and  $H(q, p)$  are polynomials in the variables  $q_i, p_j$  (as they usually are) then the brackets  $\{A, H\}$  can be calculated by repeated use of the first property. In each step one  $q_i$  or  $p_j$  is brought outside a bracket, so that at the end only the brackets of  $q_i$  and  $p_j$  are present. Once these are evaluated according to the second property, the result becomes a sum of polynomials in  $q_i, p_j$ . We will denote this specific sum of polynomials as  $S(q, p)$ , so that

$$\{A(q, p), H(q, p)\} = S(q, p)$$

⁵¹If the point masses are subject to some constraints, the whole thing becomes technically more involved. But there is no need to understand these difficulties on a first attempt to grasp the basic idea.

⁵²Achieving the Hamiltonian formulation of a given classical field theory can turn out to be less straightforward than one might expect. As the matter of fact this is the case in perhaps the most iconic example of the canonical quantization procedure, namely in obtaining the quantum electrodynamics from the well known classical limit, i. e. the Maxwell electrodynamics. We will discuss these issues in the second part of the book.

Now the same technique can be used for evaluation of the commutator  $[\hat{A}, \hat{H}]$  in the Heisenberg equations of quantum mechanics

$$i\hbar \frac{d}{dt} \hat{A}(\hat{q}, \hat{p}) = [\hat{A}(\hat{q}, \hat{p}), \hat{H}(\hat{q}, \hat{p})]$$

if the operators  $\hat{A}$  and  $\hat{H}$  are polynomials in operators  $\hat{q}_i, \hat{p}_j$  satisfying the canonical commutation relations. The point is that commutators also have the property analogous to the first property of Poisson brackets and canonical commutation relations are (up to a constant) analogous to the second property of Poisson brackets

- $[\hat{B}, \hat{C}\hat{D}] = [\hat{B}, \hat{C}]\hat{D} + \hat{C}[\hat{B}, \hat{D}] \quad [\hat{B}\hat{C}, \hat{D}] = \hat{B}[\hat{C}, \hat{D}] + [\hat{B}, \hat{D}]\hat{C}$
- $[\hat{q}_i, \hat{q}_j] = [\hat{p}_i, \hat{p}_j] = 0 \quad [\hat{q}_i, \hat{p}_j] = i\hbar\delta_{ij}$

The same line of evaluation leads us therefore to the same sum of polynomials as it did in the case of Poisson brackets

$$[\hat{A}(\hat{q}, \hat{p}), \hat{H}(\hat{q}, \hat{p})] = i\hbar \hat{S}(\hat{q}, \hat{p})$$

where  $\hat{S}$  is (up to the ordering of the operators in products) the same polynomial of  $\hat{q}, \hat{p}$  as  $S$  was of  $q, p$ . For the time evolution of the mean value one has  $i\hbar \frac{d}{dt} \bar{A} = i\hbar \overline{\hat{S}(\hat{q}, \hat{p})}$  and Taylor expanding the function  $\hat{S}(\hat{q}, \hat{p})$  around the mean values  $\bar{q}, \bar{p}$  one obtains (just like in the case of the Ehrenfest theorems)

$$\frac{d}{dt} \bar{A} = S(\bar{q}, \bar{p}) + \dots$$

where ellipsis stand for corrections proportional to variances and higher central moments of  $\hat{q}$  and  $\hat{p}$ . Without the ellipsis these generalized Ehrenfest theorems are nothing else but the truly classical equations for time evolution in the Hamiltonian formalism of classical mechanics (written in terms of Poisson brackets).

The analogy derived above between quantum and classical theories is the core of the canonical quantization procedure: to obtain a quantum theory with a given classical limit, one writes this classical limit in Hamiltonian form, then replaces the canonical variables with operators and the Poisson brackets with commutators. For now, this is all we wanted to say. In subsequent chapters we will refine and generalize this procedure in several ways. We will discuss the specification of the Hilbert space the canonically quantized operators act on, we will formulate the whole scheme for fields rather than point masses, we will generalize the scheme to incorporate fermion operators (for which the canonical relations involve anticommutators rather than commutators), and we will learn how to proceed in the case of constrained systems. All of this will turn out to be important, but right now we do not need it.

There is, however, one thing worth mentioning already here. So far we treated non-relativistic and relativistic quantum theory on the same footing. But as a matter of fact, relativity cannot be merged with quantum theory easily — it is much more complicated to build a relativistic quantum theory than it was in the non-relativistic case. Fortunately, it turns out that with the help of specific linear combinations of creation and annihilation operators (these combinations are called quantum fields) one can formulate quantum theories which are guaranteed to be relativistic. And now comes the punchline of canonical quantization in merging quantum theory with relativity: the canonical quantization of classical relativistic field theory provides exactly the quantum fields needed for the formulation of relativistic quantum theory. The keywords of the previous sentence are "quantum" and "relativistic." The former was discussed thoroughly in this section, the latter is to be discussed briefly in the next section.

## 1.3 Relativity and Quantum Theory

Actually, as to the quantum fields, the keyword is relativity. Even if QFT is useful also in the nonrelativistic context (see the previous section and the Appendix), the very notion of the quantum field originated from an endeavor to fit together relativity and quantum theory. This is a nontrivial task: to formulate a relativistic quantum theory is significantly more complicated than it is in a nonrelativistic case. The reason is that specification of a Hamiltonian, the crucial operator of any quantum theory, is much more restricted in relativistic theories.

To understand the source of difficulties, it is sufficient to realize that to have a relativistic quantum theory means to have a quantum theory with measurable predictions which remain unchanged by the relativistic transformations. The relativistic transformations at the classical level are the space-time transformations conserving the interval  $ds = \eta_{\mu\nu} dx^\mu dx^\nu$ , i.e. boosts, rotations, translations and space-time inversions (the list is exhaustive). They constitute a group.

Now to the quantum level: whenever macroscopic measuring and/or preparing devices enjoy a relativistic transformation, the Hilbert (Fock) space should transform according to a corresponding linear⁵³ transformation. It is also almost self-evident that the quantum transformation corresponding to a composition of classical transformations (at the level of macroscopic devices) should be equal to the composition of quantum transformations corresponding to the individual classical transformations. So at the quantum level the relativistic transformations should constitute a representation of the group of classical transformations.

The point now is that the Hamiltonian, as the time-translations generator, is just one of ten generators of the Poincaré group representation (the other nine are boosts, rotations, space-translations generators). Consequently, unlike in a nonrelativistic QM, in a relativistic quantum theory one cannot specify the Hamiltonian alone, one has rather to specify it within a complete representation of the Poincaré algebra. This is the starting point of any effort to get a relativistic quantum theory, even if it is not always stated explicitly. The outcome of such efforts are quantum fields. Depending on the philosophy adopted, they use to emerge in at least two different ways. We will call them particle-focused and field-focused.

The particle-focused approach, represented mostly by the Weinberg's book, is very much in the spirit of the previous section. One starts from the Fock space, which is systematically built up from the 1-particle Hilbert space. Creation and annihilation operators are then defined as very natural objects, namely as maps from the  $n$ -particle subspace into  $(n \pm 1)$ -particle ones, and only afterwards quantum fields are built from these operators in a bit sophisticated way (keywords being cluster decomposition principle and relativistic invariance).

The field-focused approach (represented by Peskin–Schroeder, and shared by the majority of textbooks on the subject) starts from the quantization of a classical field, introducing the creation and annihilation operators in this way as quantum incarnations of the normal mode expansion coefficients, and finally providing Fock space as the world for these operators to live in. The logic behind this formal development is nothing else but construction of the Poincaré group generators. So, again, the corner-stone is the relativistic invariance.

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⁵³Linearity of transformations at the quantum level is necessary to preserve the superposition principle. The symmetry transformations should not change measurable things, which would not be the case if the superposition  $|\psi\rangle = c_1 |\psi_1\rangle + c_2 |\psi_2\rangle$  would transform to  $T|\psi\rangle \neq c_1 T|\psi_1\rangle + c_2 T|\psi_2\rangle$ .

### 1.3.1 Lorentz and Poincaré groups

This is by no means a systematic exposition to the Lorentz and Poincaré groups and their representations. It is rather a summary of important relations, some of which should be familiar (at some level of rigor) from the previous courses.

#### the groups

The classical relativistic transformations constitute a group, the corresponding transformations at the quantum level constitute a representation of this group. The group transformations are

$$x^\mu \rightarrow \Lambda^\mu_\nu x^\nu + a^\mu$$

where  $\Lambda^\mu_\nu$  are combined space rotations, boosts and space-time inversions, while  $a^\mu$  describe space-time translations. The rotations around (and the boosts along) the space axes are ⁵⁴

$$\begin{aligned} R_1(\vartheta) &= \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & \cos \vartheta & -\sin \vartheta \\ 0 & 0 & \sin \vartheta & \cos \vartheta \end{pmatrix} & B_1(\beta) &= \begin{pmatrix} \text{ch } \beta & \text{sh } \beta & 0 & 0 \\ \text{sh } \beta & \text{ch } \beta & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \\ R_2(\vartheta) &= \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \cos \vartheta & 0 & \sin \vartheta \\ 0 & 0 & 1 & 0 \\ 0 & -\sin \vartheta & 0 & \cos \vartheta \end{pmatrix} & B_2(\beta) &= \begin{pmatrix} \text{ch } \beta & 0 & \text{sh } \beta & 0 \\ 0 & 1 & 0 & 0 \\ \text{sh } \beta & 0 & \text{ch } \beta & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \\ R_3(\vartheta) &= \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \cos \vartheta & -\sin \vartheta & 0 \\ 0 & \sin \vartheta & \cos \vartheta & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} & B_3(\beta) &= \begin{pmatrix} \text{ch } \beta & 0 & 0 & \text{sh } \beta \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ \text{sh } \beta & 0 & 0 & \text{ch } \beta \end{pmatrix} \end{aligned}$$

where  $\vartheta$  is the rotation angle (in counterclockwise direction) and  $\tanh \beta = v/c$  where  $v$  is the velocity of the boost. They constitute the Lorentz group. It is a non-compact (since  $\beta \in (-\infty, \infty)$ ) Lie group. The translations along the space-time axes are

$$T_0(\alpha) = \begin{pmatrix} \alpha \\ 0 \\ 0 \\ 0 \end{pmatrix} \quad T_1(\alpha) = \begin{pmatrix} 0 \\ \alpha \\ 0 \\ 0 \end{pmatrix} \quad T_2(\alpha) = \begin{pmatrix} 0 \\ 0 \\ \alpha \\ 0 \end{pmatrix} \quad T_3(\alpha) = \begin{pmatrix} 0 \\ 0 \\ 0 \\ \alpha \end{pmatrix}$$

Together with the boosts and rotations they constitute the Poincaré group. It is a non-compact Lie group (on top of the non-compactness of the Lorentz subgroup one has  $\alpha \in (-\infty, \infty)$ ). The space-time inversions are three different diagonal matrices. The time inversion is given by  $T = \text{diag}(-1, 1, 1, 1)$ , the space inversion is given by  $P = \text{diag}(1, -1, -1, -1)$  and their product is  $PT = \text{diag}(-1, -1, -1, -1)$ .

⁵⁴A comment on signs seems to be appropriate here. Transformations can be understood as active ones (transformations of objects) or passive ones (transformations of viewpoints). In the quantum mechanics we usually understand rotations and translations as active transformations within one reference frame. In the special relativity, however, we usually understand Lorentz transformations as passive transformations between two different reference frames. If the primed frame is rotated or boosted with respect to the unprimed frame then we can express the unprimed coordinates as functions of the primed ones:  $x^\mu = \Lambda^\mu_{\nu'} x^{\nu'}$ . Our choice of signs in front of  $\sin(\vartheta)$  and  $\text{sh}(\beta)$  corresponds to this choice (which, by the way, is equivalent to active transformations). If we decide to express primed coordinates as functions of unprimed, we would get opposite signs.

### the Lie algebra

The standard technique of finding representations of a Lie group is to find representations of the corresponding Lie algebra (the commutator algebra of the generators). The standard choice of the generators corresponds to the 10 types of (infinitesimal) transformations listed above: rotations  $R_i(\varepsilon) = \mathbb{1} - i\varepsilon J_i + \mathcal{O}(\varepsilon^2)$ , boosts  $B_i(\varepsilon) = \mathbb{1} - i\varepsilon K_i + \mathcal{O}(\varepsilon^2)$ , space translations⁵⁵  $T_i(\varepsilon) = -i\varepsilon P_i + \mathcal{O}(\varepsilon^2)$  and time translation⁵⁶  $T_0(\varepsilon) = i\varepsilon P_0 + \mathcal{O}(\varepsilon^2)$ .

$$J_1 = i \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 \end{pmatrix} \quad K_1 = i \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

$$J_2 = i \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{pmatrix} \quad K_2 = i \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

$$J_3 = i \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \quad K_3 = i \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}$$

$$P_0 = i \begin{pmatrix} -1 \\ 0 \\ 0 \\ 0 \end{pmatrix} \quad P_1 = i \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix} \quad P_2 = i \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix} \quad P_3 = i \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}$$

Calculation of the commutators is straightforward⁵⁷ (even if not very exciting)

$$\begin{aligned} [J_i, J_j] &= i\varepsilon_{ijk} J_k & [J_i, P_0] &= 0 \\ [J_i, K_j] &= i\varepsilon_{ijk} K_k & [J_i, P_j] &= i\varepsilon_{ijk} P_k \\ [K_i, K_j] &= -i\varepsilon_{ijk} J_k & [K_i, P_0] &= -iP_i \\ [P_\mu, P_\nu] &= 0 & [K_i, P_j] &= -iP_0 \delta_{ij} \end{aligned}$$

⁵⁵For additive group the unit element is zero (no translation at all) and therefore we have 0 instead of 1 in the definition of the translation generator.

⁵⁶The sign in the definition of this generator is plus instead of the usual minus. Such a choice of sign is a common habit in quantum mechanics and it leads to the standard relations for the space translation generators  $P_i = -i\partial_i$  (the momentum operator in the  $x$ -representation) and the time translation generator  $P_0 = i\partial_0$  i.e.  $H = i\partial_t$  (the Schrödinger equation). In the non-relativistic QM this choice of signs may look a bit weird (even if we are all used to it), but in relativity it is quite natural, since it corresponds to the relativistic relation  $P_\mu = i\partial_\mu$ . Recall that the sign of space components of a 4-vector and the 4-gradient are opposite:  $P_\mu = (P_0, -\vec{P})$ ,  $\partial_\mu = (\partial_0, \nabla)$ .

⁵⁷Commutators of  $J_i$  (or  $K_i$ ) and  $P_\mu$  follow from  $\Lambda^\mu_\nu(x^\nu + a^\nu) - (\Lambda^\mu_\nu x^\nu + a^\mu) = \Lambda^\mu_\nu a^\nu - a^\mu = (\Lambda - 1)^\mu_\nu a^\nu$ , i.e. one obtains the commutator by acting of the corresponding generator  $J_i$  or  $K_i$  on the (formal) vector  $P_\mu$ .

**Remark:** As the matter of fact (a sad one), there are multiple possibilities for choice of sign when speaking about symmetry groups and their representations. One can understand transformations in either active or passive sense (the difference being just the sign). One can use either plus or minus sign in the definition of generators  $U(\varepsilon) = \mathbb{1} \pm i\varepsilon G + \mathcal{O}(\varepsilon^2)$  (and we have already used both – one for time translations and the other one for all the others). One can, but is not obliged to, use the explicit  $i$  in this definition, which change the sign of commutators (let us note that the standard physicists's argument that with the  $i$  the generators become hermitian does not work for the Lorentz boosts, as we could notice). One can define transformations of operators either as  $A \rightarrow UAU^{-1}$  or as  $A \rightarrow U^{-1}AU$ . The first choice corresponds to simultaneous transformations of state vectors and operators, the second choice corresponds to the Heisenberg picture of transforming operators and untouched states. For infinitesimal transformations the difference is again just the sing. And one can use different signatures for Minkowski metric tensor, i.e. either  $\eta_{\mu\nu} = \text{diag}(1, -1, -1, -1)$  or  $\eta_{\mu\nu} = \text{diag}(-1, 1, 1, 1)$ . In this text we will (try to) use: active transformations,  $U(\varepsilon) = \mathbb{1} - i\varepsilon G + \mathcal{O}(\varepsilon^2)$  (with exception of the time translations),  $A \rightarrow UAU^{-1}$  and  $\eta_{\mu\nu} = \text{diag}(1, -1, -1, -1)$ .

**Remark:** The commutation relations hold for the Lie algebra as well as for its representations. For representations in Hilbert space of quantum states, the generators of time-translations, space-translations and space-rotations are energy, momentum and angular momentum operators respectively. From their commutation relations one can conclude that

1. Representations of  $J_j, K_j, P_j$  transform as components of 3-vectors.⁵⁸
2. Representations of  $P_0, P_j, J_j$  are conserved quantities (they commute with the hamiltonian).
3. Representations of  $K_j$  are not conserved (they do not commute with the hamiltonian).
4. Representations of  $P_\mu$  transform as components of 4-vector.⁵⁹
5. Representations of  $J_i$  and  $K_i$  transform as components of antisymmetric 4-tensor.⁶⁰

**Remark:** The generators of the Lorentz group are  $4 \times 4$  matrices with only non-zero elements being  $\pm i$ . Such matrices can be written using just the metric tensor  $\eta$ . As an example let us write the matrix  $(K_1)^\mu_\nu$  as  $i(\eta_1^\mu \eta_{0\nu} - \eta_0^\mu \eta_{1\nu})$ . In general one can write (as the reader should check)

$$(M_{\alpha\beta})^\mu_\nu = i \left( \eta_\alpha^\mu \eta_{\beta\nu} - \eta_\beta^\mu \eta_{\alpha\nu} \right) \quad J_k = \frac{1}{2} \varepsilon_{ijk} M_{ij} \quad K_i = M_{i0}$$

The matrices  $M_{\alpha\beta}$  are numbered by the indices  $\alpha, \beta$  and are antisymmetric in them. One can therefore write the general infinitesimal Lorentz transformation as  $\Lambda = \mathbb{1} - \frac{i}{2} \varepsilon^{\alpha\beta} M_{\alpha\beta}$  with an antisymmetric  $\varepsilon^{\alpha\beta}$ . The advantage of the matrices  $M^{\alpha\beta}$  is twofold. First, it provides a compact notation, and second, it reveals clearly the 4-tensor character of the Lorentz generators. Indeed, since  $\eta$  is the (metric) 4-tensor, the  $M$  is by definition 4-tensor with four indices (rank 4), i.e. it is a second rank tensor with respect to the indices  $\alpha$  and  $\beta$ .

⁵⁸Infinitesimal rotations of three operators  $A_j$  are given by  $(1 - i\varepsilon J_i)A_j(1 + i\varepsilon J_i) = A_j - i\varepsilon[J_i, A_j] + \mathcal{O}(\varepsilon^2)$ , which for  $A_i = J_i, K_i, P_i$  is equal to  $A_j + \varepsilon \varepsilon_{ijk} A_k + \mathcal{O}(\varepsilon^2)$  (due to the commutation relations). Components of a 3-vector  $\vec{a}$ , on the other hand, are transformed according to the defining representation of the rotation group  $\vec{a} \rightarrow (1 - i\varepsilon J_i)\vec{a}$ , which for  $(J_i)_{jk} = -i\varepsilon_{ijk}$  (in this representation), equals to  $a_j \rightarrow a_j - \varepsilon \varepsilon_{ijk} a_k + \mathcal{O}(\varepsilon^2)$ . So up to the sign the operators  $A_i = J_i, K_i, P_i$  transform as the components of a 3-vector. And since in this case the difference in the sign is just the difference between e.g. active and passive transformations, we may conclude that operators  $J_i, K_i, P_i$  do indeed transform as components of 3-vectors.

⁵⁹Infinitesimal Lorentz transformations of four operators  $P_\mu$  are  $(1 - i\varepsilon J_i)P_\mu(1 + i\varepsilon J_i) = P_\mu - i\varepsilon[J_i, P_\mu] + \mathcal{O}(\varepsilon^2)$  and  $(1 - i\varepsilon K_i)P_\mu(1 + i\varepsilon K_i) = P_\mu - i\varepsilon[K_i, P_\mu] + \mathcal{O}(\varepsilon^2)$ . Components of a 4-vector  $a_\mu$  are transformed according to the defining representation of the Lorentz group  $a \rightarrow (1 - i\varepsilon J_i)a$  and  $a \rightarrow (1 - i\varepsilon K_i)a$ . The commutators (in general) and the generators in the defining representation are given explicitly at the previous page, from where one can conclude (just like in the previous footnote) that indeed up to the sign the operators  $P_\mu$  transform as the components of a 4-vector.

⁶⁰This should be clear from the last remark on this page.

### 1.3.2 The scalar representation of the Poincaré group

Representations of the Poincaré group are of vital importance to any serious attempt to discuss relativistic quantum theory. It is, however, not our task right now. For quite some time we will need only the simplest representation – the so-called scalar one, which is quite easy to guess (and that's what we are going to do now). Systematic analysis of representations of the Lorentz and Poincaré groups and all the complications introduced by non-scalar representations are postponed to next chapters.

Let us consider a Hilbert space in which some representation of the Poincaré group is defined. Perhaps the most convenient basis of such a space is the one defined by the eigenvectors of the representations of the translation generators  $\mathcal{P}_\mu$ , commuting with each other. The eigenvectors are usually denoted as  $|p, \sigma\rangle$ , where  $p = (p_0, p_1, p_2, p_3)$  stands for eigenvalues of  $\mathcal{P}$  and  $\sigma$  stands for any other quantum numbers. In this notation  $\mathcal{P}_\mu |p, \sigma\rangle = p_\mu |p, \sigma\rangle$ .

At this point we are going to consider only the simplest case, the so-called scalar representation, in which no  $\sigma$  is involved. The states in this representation are characterized completely by the 4-momentum  $p$ , which is exactly what one expects to be the case for one spinless particle. For the translation generators in this representation one has

$$\mathcal{P}_\mu |p\rangle = p_\mu |p\rangle$$

The representation of non-infinitesimal space-time translations  $x \rightarrow x + a$  is obtained by exponentialization of the generators

$$|p\rangle \xrightarrow{a} e^{-ia^\mu \mathcal{P}_\mu} |p\rangle = e^{-ia^\mu p_\mu} |p\rangle$$

How does the representation of the Lorentz transformations  $x \rightarrow \Lambda x$  look like? Since  $p$  is a 4-vector, the obvious first guess is to simply transform it correspondingly (a state characterized by a momentum is transformed to the state characterized by the Lorentz transformed momentum)

$$|p\rangle \xrightarrow{\Lambda} |\Lambda p\rangle$$

It is straightforward to check (do it) that this, indeed, is a representation of the Lorentz group. Finally one puts the Lorentz transformations and translations together to get

$$|p\rangle \xrightarrow{\Lambda, a} U(\Lambda, a) |p\rangle = e^{-i(\Lambda p)^\mu a_\mu} |\Lambda p\rangle$$

where  $U(\Lambda, a)$  is the representation of the transformation  $x \rightarrow \Lambda x + a$  and  $(\Lambda p)^\mu a_\mu = \Lambda_\mu^\nu p_\nu a^\mu$ . It is again easy to check directly (do it) that this defines a representation of the Poincaré group.⁶¹

Once we have a Poincaré group representation it is straightforward to obtain the representation of the Poincaré algebra

$$\mathcal{P}_\mu |p\rangle = p_\mu |p\rangle \quad \mathcal{J}_i |p\rangle = |J_i p\rangle \quad \mathcal{K}_i |p\rangle = |K_i p\rangle$$

The time translations generator  $\mathcal{P}_0$  is the Hamiltonian, the space translations generators  $\mathcal{P}_i$  are the momentum operators and the space rotations generators  $\mathcal{J}_i$  are the angular momentum operators.

⁶¹Hint: At some point it may come handy to realize that  $(\Lambda v)(\Lambda w) = vw$ , i. e.  $(\Lambda \Lambda' p)(\Lambda a') = (\Lambda' p)a'$ . Let us remark that once the spin is involved, the parameter  $\sigma$  enters the game and the transformation is a bit more complicated. It goes like this:  $U(\Lambda, a) |p, \sigma\rangle = \sum_{\sigma'} e^{-i(\Lambda p)^\mu a_\mu} C_{\sigma\sigma'} |\Lambda p, \sigma'\rangle$  and the coefficients  $C_{\sigma\sigma'}$  define the particular representation of the Lorentz group. These complications, however, do not concern us now. For our present purposes the simplest scalar representation will be sufficient.

We have obtained one particular representation of the Poincaré group, i.e. we have at our disposal one specific relativistic quantum theory. To what physical system does this theory correspond? To get the answer it is useful to realise that the operator  $P^2 = P_\mu P^\mu$  commutes with all the generators of the Poincaré group (check it), i.e. it is a Casimir operator of this group. In any irreducible representation the corresponding operator  $\mathcal{P}^2$  is proportional to the identity operator (Schur's lemma). Let's denote the proportionality constant  $m^2$ . For all basis states  $|p\rangle$  in the irreducible representation one has

$$\mathcal{P}^2 |p\rangle = (E^2 - \vec{p}^2) |p\rangle = m^2 |p\rangle$$

so in every irreducible representation only three out of four components of  $p$  are independent. It is a common habit to consider components of  $\vec{p}$  independent and to demand  $p^0 = \sqrt{\vec{p}^2 + m^2}$ . This defines the hamiltonian unambiguously as⁶²

$$H |p\rangle = \mathcal{P}_0 |p\rangle = \sqrt{\vec{p}^2 + m^2} |p\rangle$$

So our irreducible representation is just what one would expect from the Hilbert space of quantum states of free spinless relativistic particle with the mass  $m$ .

In spite of looking fairly simple, our representation of the Poincaré group contains a couple of tricky issues – some of them just technical, others quite deep. One of the technical issues is the normalization of states. The standard normalization condition using the  $\delta$ -function is not relativistic invariant. Indeed, the integral  $\int d^3p \delta^3(\vec{p}) = 1$  is invariant (it is constant by definition), while  $d^3p$  and  $\delta^3(\vec{p})$  individually are not ( $d^3p$  due to the Lorentz contraction,  $\delta^3(\vec{p})$  as a consequence). The ratio  $d^3p/E$ , however, is invariant⁶³ and as a consequence so is the product  $E \delta^3(\vec{p})$ . It is therefore a common habit in relativistic quantum theory to use the Lorentz invariant normalization condition⁶⁴

$$\langle p | p' \rangle = (2\pi)^3 2E_{\vec{p}} \delta^3(\vec{p} - \vec{p}')$$

where  $E_{\vec{p}} = p_0 = \sqrt{\vec{p}^2 + m^2}$ . One should keep this normalization in mind when using various identities known from the standard non-relativistic QM. As an example let us mention the identity operator expressed in terms of  $|\vec{p}\rangle \langle \vec{p}|$ . Instead of the non-relativistic expression⁶⁵  $1 = \int d^3p |\vec{p}\rangle \langle \vec{p}|$  the correct relativistic expression (with the relativistic normalization defined above) reads

$$1 = \int \frac{d^3p}{(2\pi)^3 2E_{\vec{p}}} |p\rangle \langle p|$$

The combination  $\frac{d^3p}{(2\pi)^3 2E_{\vec{p}}}$  is so common in relativistic quantum theory that it has its own name. It is called "infinitesimal Lorentz invariant phase space", sometimes abbreviated as dLIPS.

⁶²Let us emphasize that it is the specific choice of an irreducible representation (the choice of  $m$ ) that determines the Hamiltonian. Before this choice our representation of the Poincaré algebra did not provide any specific Hamiltonian, it just states that the Hamiltonian is the generator of the time translations. After the choice, however, the Hamiltonian is fixed, no freedom was left.

⁶³Indeed, let us consider the boost along the  $x_3$  axis, with the velocity  $\beta$ . The Lorentz transformation of a 4-momentum  $p = (E, \vec{p})$  is  $E \rightarrow \gamma E + \gamma \beta p_3$ ,  $p_1 \rightarrow p_1$ ,  $p_2 \rightarrow p_2$  and  $p_3 \rightarrow \gamma p_3 + \gamma \beta E$  (where  $\gamma = \sqrt{1 - \beta^2}$ ), and the same transformation holds for an infinitesimal 4-vector  $dp$ . Clearly,  $d^3p$  is not invariant  $d^3p \rightarrow dp_1 dp_2 (\gamma dp_3 + \gamma \beta dE) = d^3p (\gamma + \gamma \beta dE/dp_3)$ . For  $dE = 0$  this would be just a Lorentz contraction, but if both  $p$  and  $p + dp$  correspond to the same mass  $m$ , then  $E = \sqrt{m^2 + \vec{p}^2}$  and  $dE/dp_3 = p_3/\sqrt{m^2 + \vec{p}^2} = p_3/E$ . Therefore  $d^3p \rightarrow d^3p (\gamma + \gamma \beta p_3/E)$  and finally  $\frac{d^3p}{E} \rightarrow \frac{d^3p (\gamma + \gamma \beta p_3/E)}{\gamma E + \gamma \beta p_3} = \frac{d^3p}{E}$ .

⁶⁴The factor  $(2\pi)^3$  was discussed already at the page 26, the convenience of the extra factor of 2 (i. e. the reason for  $2E$  instead of  $E$ ) will become clear later.

⁶⁵The symbol  $|\vec{p}\rangle$  is used for the states normalized to the  $\delta$ -function (see page 26), i. e.  $|p\rangle = \sqrt{(2\pi)^3 2E_{\vec{p}}} |\vec{p}\rangle$ .

**note on localized states**

And now for a deeper issue with our representation of the Poincaré group. The states  $|p\rangle$  with sharp values of four-momentum constitute a natural and convenient basis for our representation. One might assume the same to be true for states strictly localized in space-time. Such states, however, are notoriously known to be problematic in relativistic quantum theories.

The problem is not that these states are not well defined. The spatially localized states  $|\vec{x}\rangle$  can be defined just as in non-relativistic quantum mechanics

$$|\vec{x}\rangle = \int d^3p |\vec{p}\rangle \langle \vec{p} | \vec{x} \rangle = \int \frac{d^3p}{\sqrt{(2\pi)^3}} e^{-i\vec{p}\cdot\vec{x}} |\vec{p}\rangle$$

Now let us assume this to be the state of the particle at  $t = 0$  and let us denote this state as  $|x\rangle_{NW}$  with  $x^0 = 0$  (the subscript stands for Newton and Wigner, who considered such states explicitly within relativistic quantum theory). For such a state one has  $px = p^0 0 - \vec{p} \cdot \vec{x}$ , i. e.

$$|x\rangle_{NW} = \int \frac{d^3p}{(2\pi)^3 \sqrt{2E_{\vec{p}}}} e^{ipx} |p\rangle$$

There is nothing wrong with this state from the quantum point of view. It is, however, quite a troublemaker from the relativistic point of view.

Let us start with the Lorentz transformations. One could naively (but incorrectly) expect a transformation similar to that of the  $|p\rangle$  states, i. e.  $|x\rangle_{NW} \xrightarrow{\Lambda} |\Lambda x\rangle_{NW}$ . But this turns out not to be the case. Indeed, it is straightforward to write down the state into which  $|x\rangle_{NW}$  is transformed – one just has to take the definition of  $|x\rangle_{NW}$  and replace every state  $|p\rangle$  by  $|\Lambda p\rangle$  (the transformed state is the same superposition of the transformed momentum eigenstates)

$$|x\rangle_{NW} \xrightarrow{\Lambda} \int \frac{d^3p}{(2\pi)^3 \sqrt{2E_{\vec{p}}}} e^{ipx} |\Lambda p\rangle$$

The state  $|\Lambda x\rangle_{NW}$ , on the other hand, is trivially obtained by the replacement  $x \rightarrow \Lambda x$  in the definition of  $|x\rangle_{NW}$

$$|\Lambda x\rangle_{NW} = \int \frac{d^3p}{(2\pi)^3 \sqrt{2E_{\vec{p}}}} e^{ip\Lambda x} |p\rangle$$

After the substitution  $p \rightarrow \Lambda p$ , the product of the exponent and the state vector in the integral becomes  $e^{ipx} |\Lambda p\rangle$ , i. e. exactly the same structure which is present in the previous integral. This substitution, however, changes the remaining term  $\frac{d^3p}{(2\pi)^3 \sqrt{2E_{\vec{p}}}}$  (were it not for the square root in the denominator, this term would be invariant⁶⁶ – with the square root, it is not). The integrals are therefore not equal, and one can conclude that

$$|x\rangle_{NW} \not\xrightarrow{\Lambda} |\Lambda x\rangle_{NW}$$

The problem with the (Newton–Wigner) strictly localized states in relativistic quantum theory (or at least in our scalar representation) is not that they do not make sense, but rather that they are not decent relativistic notions. A state perceived by one inertial observer as strictly local is not perceived as strictly local by other inertial observers moving with respect to the first one.

⁶⁶This seemingly innocuous statement will turn out to be very important later on. It asserts that, unlike  $|x\rangle_{NW}$ , a different state  $|x\rangle_{abnql} = \int \frac{d^3p}{(2\pi)^3 \sqrt{2E_{\vec{p}}}} e^{ipx} |p\rangle$  transforms in a perfectly relativistic way:  $|x\rangle_{abnql} \xrightarrow{\Lambda} |\Lambda x\rangle_{abnql}$  (the subscript *abnql* stands for "almost but not quite localized" – for the proof of this property see Appendix ??). Such states are going to play a crucial role in QFT as a neat compromise between localizability and relativity.

Strictly localized NW states are problematic not only under Lorentz transformations, but also under time translations. To see this, let us consider translated NW state

$$|x\rangle_{NW} \xrightarrow{a} \int \frac{d^3p}{(2\pi)^3 \sqrt{2E_{\vec{p}}}} e^{ipx} e^{-ipa} |p\rangle$$

For purely spatial translation this represents no problem:  $|x\rangle_{NW} \xrightarrow{(0,\vec{a})} |x-a\rangle_{NW}$  so the new state is just the original state shifted by  $-\vec{a}$  (at the time  $x^0 = 0$ ). For time translations, however, one encounters an unpleasant surprise: for any  $t > 0$  the time-evolved state has non-vanishing overlap with position eigenstates  $|y\rangle_{NW}$  outside the forward light-cone (the proof can be found in Appendix B or in Coleman's book, pp. 12-14). This means superluminal signal propagation, which is almost inevitably in conflict with causality.⁶⁷

The usual textbook interpretation of the above-mentioned clash between localizability and causality goes something like this: 1-particle relativistic quantum theory is not causal, and one is therefore forced to promote it to a multiparticle quantum theory. This mysterious claim seems to imply that, in the multi-particle formulation, the problem somehow disappears. This, however, is simply not true. For particles without interactions, the 1-particle subspace of the Fock space is just the free 1-particle Hilbert space equipped with the same free Hamiltonian — so any pathology of the one-particle theory is necessarily present also in the one-particle sector of the multi-particle free theory.

Without delving too deeply into the localizability problem in relativistic quantum theory, let us at least comment on some of its aspects. First of all, the problem would disappear if the states leading to superluminal signal propagation could not be prepared experimentally. Can a relativistic quantum theory be formulated in such a way that it does not allow for the experimental preparation of the "problematic" states? Yes, this can be achieved both in the one-particle and multi-particle theories. In the multi-particle case, however, the restriction to non-problematic states can be formulated in a much more physically motivated way.⁶⁸

The need for a multi-particle theory is therefore much more sophisticated than it may appear from standard expositions of the subject. But even if one is not forced to move from a one-particle theory to a multi-particle one, it is natural to do so, at least in the case of theories of elementary particles (for the simple reason that particles are frequently created and annihilated in this realm of physics). So our next step is to formulate a relativistic quantum theory in the Fock space. The simplest such theory will turn out to be just a straightforward generalization of our single-particle theory. More involved (and far more interesting) generalizations are postponed to the next chapters.

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⁶⁷Let us emphasize that the problem is not the superluminal velocity as such, but rather the superluminal velocity of signal propagation. As is well known, the phase velocity of the de Broglie wave corresponding to a free relativistic particle with four-momentum  $p$  is  $v_p = \frac{\omega}{k} = \frac{E}{|\vec{p}|} = \frac{\sqrt{\vec{p}^2 + m^2}}{|\vec{p}|} > 1$ . But since the particle with sharp momentum is omnipresent, this is not the velocity of any signal propagation. What really matters is particle propagation, which – according to the standard lore – is given by  $v_g = \frac{\partial \omega}{\partial k} = \frac{\partial E}{\partial |\vec{p}|} = \frac{\partial \sqrt{\vec{p}^2 + m^2}}{\partial |\vec{p}|} = \frac{|\vec{p}|}{\sqrt{\vec{p}^2 + m^2}} < 1$ . The standard argument leading to the notion of group velocity is, however, a bit handwavy. In Appendix ?? the loose reasoning is replaced with an actual propagation calculation. The result is superluminal propagation of the probability density, which could in principle be exploited to send a superluminal signal.

⁶⁸The trick is to admit only those states that are generated by local interactions with external sources. One can show that this trick works in the multi-particle theory but fails in the one-particle theory. This is the real difference between one-particle and multi-particle relativistic quantum physics from the causality point of view.

But there is yet another issue concerning causality present in multi-particle theories with a restricted set of experimentally achievable states. In a causal theory, measurements performed in some spacetime region cannot affect measurements in another spacelike separated region. This is not guaranteed for any theory formulated within a representation of the Poincaré group in the Fock space. But it is guaranteed for theories formulated in terms of specific linear combinations of creation and annihilation operators. These combinations are called relativistic quantum fields and we have already encountered them when discussing our toy model of quantum electrodynamics (see page 47), even if we did not use their proper name. In the rest of this paragraph, the relativistic quantum fields will appear (for different reasons) a few more times.

If one starts with the relativistic classical theory for the field  $\varphi$  in Minkowski space, then (as we will witness later) the canonical quantization will automatically provide the operators  $\varphi_{\vec{x}}$  and  $\pi_{\vec{x}}$  from page 47. These operators (called relativistic quantum fields) are not only some weird combinations of creation and annihilation operators emerging in our toy model, but essential quantities of relativistic quantum theory obtained by canonical quantization.

### the scalar representation in the Fock space

After mentioning the advantages of the multi-particle case over the one-particle one, let us promote our system of one free relativistic particle to a system of many free relativistic particles. All that is needed is to construct the Fock space starting from the one-particle Hilbert space. Such a space is spanned by the orthonormal basis

$$|0\rangle \quad |\vec{p}\rangle \quad |\vec{p}, \vec{p}'\rangle \quad \dots$$

or by the orthogonal relativistically normalized basis

$$|0\rangle \quad |p\rangle = \sqrt{(2\pi)^3 2E_{\vec{p}}} |\vec{p}\rangle \quad |p, p'\rangle = \sqrt{(2\pi)^3 2E_{\vec{p}}} \sqrt{(2\pi)^3 2E_{\vec{p}'}} |\vec{p}, \vec{p}'\rangle \quad \dots$$

Having a representation of the Poincaré generators acting in the single particle space, one trivially obtains a representation also in the corresponding Fock space – one simply transforms Fock space basis vectors by transforming the four-momenta just like in the single particle case (this is nothing else but the direct sum of the direct products of one-particle generators)

$$|p_1, \dots, p_n\rangle \xrightarrow{\Lambda, a} e^{-ia \sum_j \Lambda p_j} |\Lambda p_1, \dots, \Lambda p_n\rangle$$

For a given basis in the Fock space one can define the creation and annihilation operators in the standard way. It is a common habit to use the operators  $a_{\vec{p}}^+$  and  $a_{\vec{p}}$  (see page 26) which do not generate relativistically normalized states  $|p\rangle$ , but rather the non-relativistically normalized states  $|\vec{p}\rangle$ . For these operators one has

$$|\vec{p}\rangle = a_{\vec{p}}^+ |0\rangle \quad |\vec{p}, \vec{p}'\rangle = a_{\vec{p}}^+ a_{\vec{p}'}^+ |0\rangle \quad \dots$$

and as a consequence

$$|p\rangle = \sqrt{(2\pi)^3 2E_{\vec{p}}} a_{\vec{p}}^+ |0\rangle \quad |p, p'\rangle = \sqrt{(2\pi)^3 2E_{\vec{p}}} \sqrt{(2\pi)^3 2E_{\vec{p}'}} a_{\vec{p}}^+ a_{\vec{p}'}^+ |0\rangle \quad \dots$$

The Fock space generators can be naturally written in terms of these creation and annihilation operators as⁶⁹

$$\mathcal{P}_\mu = \int d^3p \, p_\mu a_p^+ a_p \quad \mathcal{J}_i = \int d^3p \, a_{J_i p}^+ a_p \quad \mathcal{K}_i = \int d^3p \, a_{K_i p}^+ a_p$$

Let us emphasize that it is the specific choice of an irreducible representation (the choice of  $m$ ) that determines the Hamiltonian

$$H = \mathcal{P}_0 = \int d^3p \, \sqrt{\vec{p}^2 + m^2} a_{\vec{p}}^+ a_{\vec{p}}$$

With this Hamiltonian, we have finally achieved a relativistic quantum theory of non-interacting particles with mass  $m$ . This, however, is not a very exciting system — not much physics is going on there. The question therefore is how to add some interaction to this system in a relativistic way. And this turns out to be a surprisingly difficult task.

⁶⁹It is straightforward to check this by evaluating the linear part of the infinitesimal Poincaré transformations. The results are exactly what one would expect. For translations we got the four-momentum operator of the ideal gas, for Lorentz transformations we got operators annihilating particles in the original states labeled by  $p$  and creating them in the transformed states labeled by  $J_i p$  and  $K_i p$ .

As mentioned at the end of page 50, the basic building blocks of relativistic quantum theories are not creation and annihilation operators themselves, but rather some specific linear combinations thereof. These combinations are called relativistic quantum fields, and we have already encountered them when discussing our toy model of quantum electrodynamics (see page 47), even if we did not use their proper name.

At this point it is worth noting that they appear naturally in relativistic quantum theory in the Fock space also in connection with almost but not quite localized states introduced in the footnote on page 57. Indeed, if one wants to create such a state from the vacuum state, then the operator doing the job is obvious

$$|x\rangle_{abnql} = \int \frac{d^3p}{(2\pi)^3 2E_{\vec{p}}} e^{ipx} |p\rangle = \int \frac{d^3p}{(2\pi)^{3/2}} \frac{1}{\sqrt{2E_{\vec{p}}}} e^{ipx} a_{\vec{p}}^+ |0\rangle$$

This operator, however, is not hermitian, and if one wants to deal with hermitian operators, one just add the hermitian conjugate to obtain the so-called free scalar field operator

$$\varphi(x) = \int \frac{d^3p}{(2\pi)^{3/2}} \frac{1}{\sqrt{2E_{\vec{p}}}} \left( e^{ipx} a_{\vec{p}}^+ + e^{-ipx} a_{\vec{p}} \right)$$

which for  $x^0 = 0$  is precisely the operator  $\varphi_{\vec{x}}$  from page 47.

### 1.3.3 The basic logic(s) of QFT

#### the logic of the particle-focused approach to QFT

The relativistic quantum theory describes, above all, the physics of elementary particles. Therefore the particle-focused approach looks like the most natural. Nevertheless, it is by far not the most common, for reasons which are mainly historical. Now we have to confess (embarrassed) that in these lectures we are going to follow the less natural, but more wide-spread field-focused approach.⁷⁰ The particle-focused approach is only very briefly sketched in this paragraph. *Not everything should and could be understood here, it is sufficient just to catch the flavor.* If too dense and difficult (as it is) the paragraph should be skipped.

One starts with an irreducible representation of the Poincaré group on some 1-particle Hilbert space. The usual basis vectors in the Hilbert space are of the form  $|p, \sigma\rangle$ , where  $p$  is the (overall) momentum of the state and all the other characteristics are included in  $\sigma$ . For a multiparticle state, the  $\sigma$  should contain a continuous spectrum of momenta of particular particles. This provides us with a natural definition of 1-particle states as the ones with discrete  $\sigma$ . In this case it turns out that values of  $\sigma$  correspond to spin (helicity) projections.

Irreducible representations are characterized by eigenvalues of two Casimir operators (operators commuting with all generators), one of them being  $m^2$ , the eigenvalue of the Casimir operator  $P^2$ , and the second one having to do with the spin. The states in the Hilbert space are therefore characterized by eigenvalues of 3-momentum, i.e. the notation  $|\vec{p}, \sigma\rangle$  is more appropriate than  $|p, \sigma\rangle$  (nevertheless, when dealing with Lorentz transformations, the  $|p, \sigma\rangle$  notation is very convenient). The  $|\vec{p}, \sigma\rangle$  states are still eigenstates of the Hamiltonian, with the eigenvalues  $E_{\vec{p}} = \sqrt{\vec{p}^2 + m^2}$ .

Once a representation of the Poincaré group on a 1-particle Hilbert space is known, one can systematically build up the corresponding Fock space from direct products of the Hilbert ones. The motivation for such a construction is that this would be a natural framework for processes with nonconserved numbers of particles, and such processes are witnessed in the nature. This Fock space benefits from having a natural representation of Poincaré group, namely the one defined by the direct products of the representations of the original 1-particle Hilbert space. The Hamiltonian constructed in this way, as well as all the other generators, correspond to a system of noninteracting particles. In terms of creation and annihilation operators, which are defined as very natural operators in the Fock space the free Hamiltonian has a simple form  $H_0 = \int \frac{d^3p}{(2\pi)^3} E_{\vec{p}} a_{\vec{p}}^+ a_{\vec{p}}$ .

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⁷⁰The explanation for this is a bit funny.

As to what we call here the particle-centered approach, the textbook is the Weinberg's one. We strongly recommend it to the reader, even if it would mean that he/she will quit these notes. The present author feels that he has nothing to add to the Weinberg's presentation.

But even if the approach of the Weinberg's book is perhaps more natural than any other, it is certainly not a good idea to ignore the traditional development, which we call here the field-centered approach. If for nothing else, then simply because it is traditional and therefore it became a part of the standard background of the majority of particle physicists.

Now as to the textbooks following the traditional approach, quite a few are available. But perhaps in all of them there are points (and unfortunately not just one or two) which are not explained clearly enough, and are therefore not easy to grasp (the wonderful exception is the Coleman's book, which is perhaps the best one on the subject). The aim of the present notes is to provide the standard material with perhaps a bit more emphasis put on some points which are often only glossed over. The hope is, that this would enable reader to penetrate into the subject in combination of a reasonable depth with a relative painlessness.

Nevertheless, beyond any doubt, this hope is not to be fulfilled. The reader will surely find a plenty of disappointing parts in the text.

The next step, and this is the hard one, is to find another Hamiltonian which would describe, in a relativistic way, a system of interacting particles. One does not start with a specific choice, but rather with a perturbation theory for a generic Hamiltonian  $H = H_0 + H_{\text{int}}$ . The perturbation theory is neatly formulated in the interaction picture, where  $|\psi_I(t)\rangle = U(t, 0)|\psi_I(0)\rangle$ , with  $U(t, 0)$  satisfying  $i\partial_t U(t, 0) = H_{\text{int},I}(t)U(t, 0)$  with the initial condition  $U(0, 0) = 1$ . The perturbative solution (well, in fact the iterative solution) of this equation leads to the sum of integrals of the form  $\int_{t_0}^t dt_1 \dots dt_n T H_{\text{int},I}(t_1) \dots H_{\text{int},I}(t_n)$ , where  $T$  orders the factors with respect to decreasing time. For a relativistic theory, these integrals should better be Lorentz invariant, otherwise the scalar products of the time-evolved states would be frame dependent. This presents nontrivial restrictions on the interaction Hamiltonian  $H_{\text{int}}$ . First of all, the space-time variables should be treated on the same footing, which would suggest an interaction Hamiltonian of the form  $H_{\text{int}} = \int d^3x \mathcal{H}_{\text{int}}$  and  $\mathcal{H}_{\text{int}}$  should be a Lorentz scalar. Furthermore, the  $T$ -ordering should not change the value of the product when going from frame to frame, which would suggest  $[\mathcal{H}_{\text{int}}(x), \mathcal{H}_{\text{int}}(y)] = 0$  for  $(x - y)^2 \leq 0$  (for time-like intervals, the ordering of the Hamiltonians in the  $T$ -product is the same in all the reference frames, for space-like intervals the ordering is frame-dependent, but becomes irrelevant for Hamiltonians commuting with each other).

All these requirements do not have a flavor of rigorous statements, they are rather simple observations about how could (would) a relativistic quantum theory look like. It comes as a kind of surprise, that the notion of quantum fields is a straightforward outcome of these considerations. Without going into details, let us sketch the logic of the derivation:

1. As any linear operator, the Hamiltonian can be written as a sum of products of the creation and annihilation operators. The language of the  $a_{\vec{p}}^{\pm}$  and  $a_{\vec{p}}$  operators is technically advantageous, e.g. in the formulation of the so-called cluster decomposition principle, stating that experiments which are sufficiently separated in space, have unrelated results.
2. Poincaré transformations of  $a_{\vec{p}}^{\pm}$  and  $a_{\vec{p}}$  (inherited from the transformations of states) are given by  $\vec{p}$ -dependent matrices, and so the products of such operators (with different momenta) have in general complicated transformation properties. One can, however, combine the  $a_{\vec{p}}^{\pm}$  and  $a_{\vec{p}}$  operators into simply transforming quantities called the creation and annihilation fields  $\varphi_l^+(x) = \sum_{\sigma} \int d^3p u_l(x, \vec{p}, \sigma) a_{\vec{p}}^{\sigma}$  and  $\varphi_l^-(x) = \sum_{\sigma} \int d^3p v_l(x, \vec{p}, \sigma) a_{\vec{p}, \sigma}$ , which are much more suitable for a construction of relativistic quantum theories.
3. The required simple transformation properties of  $\varphi_l^{\pm}$  are the ones independent of any  $x$  or  $\vec{p}$ , namely  $\varphi_l^{\pm}(x) \rightarrow \sum_{l'} D_{ll'}(\Lambda^{-1}) \varphi_{l'}^{\pm}(x)(\Lambda x + a)$ , where the  $D$  matrices furnish a representation of the Lorentz group. The coefficients  $u_l$  and  $v_l$  are calculable for any such representation, e.g. for the trivial one  $D_{ll'}(\Lambda^{-1}) = 1$  one gets  $u(x, \vec{p}, \sigma) = \frac{1}{(2\pi)^3 \sqrt{2E_{\vec{p}}}} e^{ipx}$  and  $v(x, \vec{p}, \sigma) = \frac{1}{(2\pi)^3 \sqrt{2E_{\vec{p}}}} e^{-ipx}$ .
4. One can easily construct a scalar  $\mathcal{H}_{\text{int}}(x)$  from the creation and annihilation fields. The vanishing commutator of two such  $\mathcal{H}_{\text{int}}(x)$  for time-like intervals, however, is not automatically guaranteed. But if  $\mathcal{H}_{\text{int}}(x)$  is constructed from a specific linear combination of the creation and annihilation fields, namely from the fields  $\varphi_l(x) = \varphi_l^+(x) + \varphi_l^-(x)$ , then the commutator is really zero for time-like intervals. This is the way how the quantum fields are introduced in the Weinberg's approach — as (perhaps the only) the natural objects for construction of interaction Hamiltonians leading to relativistic quantum theories.

### the logic of the field-focused approach to QFT

The basic idea of the field-focused approach to quantum fields is to take a classical relativistic field theory and to quantize it canonically (the exact meaning of this statement is to be explained in the next chapter). This makes a perfect sense in case of the electromagnetic field, since the primary task of the canonical quantization is to provide a quantum theory with a given classical limit. If the field is classically well known, but one suspects that there is some underlying quantum theory, then the canonical quantization is a handy tool.

This tool, however, is used also for quantum fields for which there is no such thing as the corresponding classical fields, at least not one observed normally in the nature (the electron-positron field is perhaps the prominent example). This may sound even more surprising after one realizes that there is a well known classical counterpart to the quantum electron, namely the classical electron. So if one is really keen on the canonical quantization, it seems very natural to quantize the (relativistic) classical mechanics of the electron particle, rather than a classical field theory of non-existing classical electron field. But still, what is quantized is indeed the classical field. What is the rationale for this?

First, let us indicate why one avoids the quantization of relativistic particles. Actually even for free particles this would be technically more demanding than it is for free fields. But this is not the main reason in favor of field quantization. The point is that we are not interested in free (particles or field) theory, but rather in a theory with interaction. And while it is straightforward to generalize a relativistic classical free field theory to a relativistic classical field theory with interaction (and then to quantize it), it is quite non-trivial to do so for particles.

Second, it should be perhaps emphasized that the nickname "second quantization", which is sometimes used for the canonical quantization of fields, provides absolutely no clue as to any real reasons for the procedure. On the contrary, the nickname could be very misleading. It suggests that what is quantized is not a classical field, but rather a wave-function, which may be regarded to be the result of (the first) quantization. This point of view just obscures the whole problem and is of no relevance at all (except of, perhaps, the historical one).

So why are the fields quantized? The reason is this: In the non-relativistic quantum theories the dynamics is defined by the Hamiltonian. Important point is that any decent Hamiltonian will do the job. In the relativistic quantum theories, on the other hand, the Hamiltonian, as the time-translations generator, comes in the unity of ten generators of the Poincaré group. Not every decent Hamiltonian defines a relativistic dynamics. The reason is that for a given Hamiltonian, one cannot always supply the nine friends to furnish the Poincaré algebra. As a matter of fact, it is in general quite difficult, if not impossible, to find such nine friends. Usually the most natural way is not to start with the Hamiltonian and then to try to find the corresponding nine generators, but to define the theory from the beginning by presenting the whole set of ten generators⁷¹. This is definitely much easier to say than to really provide. And here comes the field quantization, a clever trick facilitating simultaneous construction of all ten Poincaré generators.

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⁷¹From this it should be clear that even the formulation, not to speak about solution, of the relativistic quantum theory is about 10 times more difficult than that of non-relativistic quantum theory. The situation is similar to the one in general relativity with 10 components of the metric tensor as opposed to one potential describing the Newtonian gravity.

The starting point is a relativistic classical field theory. This means, first of all, that the Poincaré transformations of the field are well defined (as an example we may take the function  $\varphi(x)$  discussed on p. ??, which is now treated as a classical field transforming according to the scalar representation⁷² of the Poincaré group). Then only theories which are symmetric under these transformations are considered. Now one could expect that, after the canonical quantization, the Poincaré transformations of classical fields become somehow the desired Poincaré transformations of the Hilbert space of states. The reality, however, is a bit more sophisticated. Here we are going to sketch it only very briefly, details are to be found in the next chapter.

At the classical level, to each symmetry there is a conserved charge (Noether's theorem). When formulated in the Hamiltonian formalism, the Poisson brackets of these charges obey the same algebra, as do the Poincaré generators. After canonical quantization, the Noether charges become operators (in the Hilbert space of states), the Poisson brackets become commutators, and the Poisson bracket algebra becomes the Poincaré algebra itself (or, strictly speaking, some representation of the Poincaré algebra). Consequently, the Noether charges become, in the process of the canonical quantization, the generators of the symmetry at the quantum level.

Precisely this is going to be the logic behind the field quantization adopted in these lecture notes: field quantization is a procedure leading in a systematic way to a quantum theory with a consistent package of the ten Poincaré generators.

Let us emphasize once more that another important aspect of canonical quantization, namely that it leads to a quantum theory with a given classical limit, is not utilized here. We ignore this aspect on purpose. In spite of the immense role it has played historically and in spite of the undisputed importance of this aspect in the case of the electromagnetic field, for other fields it is illusory and may lead to undue misconceptions.

To summarize: Enlightened by the third introduction (Relativity and Quantum Theory) we are now going to penetrate a bit into the technique of the canonical quantization of relativistic classical fields. The result will be a relativistic quantum theory in terms of creation and annihilation operators familiar from the second introduction (Many-Body Quantum Mechanics). Clever version of the perturbation theory formulated within the obtained theories will then lead us to the Feynman rules discussed in the first introduction (Conclusions).

### the logic of the amplitude-focused approach to QFT

For the sake of completeness, let us mention yet another approach to quantum field theory — the one which can be naturally called the amplitude-focused approach, but is usually referred to as the path-integral approach. We will treat this approach (in chapter ??) mainly as a handy bookkeeping device for the previous two approaches. It can, however, also be used for the definition of QFT from the very beginning. On top of being a nice bookkeeping tool, this approach enables a couple of insights into matters which look much more complicated in the other two approaches.

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⁷²Why representation, why not any (possibly non-linear) realization? We have answered this question (the keyword was the superposition principle) supposing realization in the Hilbert space of quantum states. Now  $\varphi(x)$  does not correspond to the quantum state, so it is legitimate to raise the question again.

The answer (pretty unclear at the moment) is that non-linear transformations of classical fields would lead, after quantization, to transformations not conserving the number of particles, which is usually "unphysical" in a sense that one could discriminate between two inertial systems by counting particles.