Quantum Physics

At Any Cost

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Quantum Physics At Any Cost
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To the Great and Beautiful Nation
Which Gave Me Everything and More:
A Shelter, Opportunities and Inspiration,
And The Desire To Explore

Contents

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My friends, discussing the book with you was both illuminating and fun.

Finally, special acknowledgment must be given to my son, Daniel, for his help with fixing colors in many figures.

Yury Deshko
Weehawken, New Jersey
2024

Preface

This book is the result of lectures delivered to curious, motivated, and studious high schoolers. The lectures ran during the years 2019-2024 in various formats, but mostly in class during a three week summer school organized by Columbia University Pre-College Programs. Additionally, the same lectures were taught remotely to selected students of Ukrainian Physics and Mathematics Lyceum.

The material has been designed to be accessible to people with solid background in high-school algebra and physics (mostly mechanics). Several years of teaching to a relatively diverse set of students proved that nearly all material can be efficiently absorbed by most, provided diligent work is done on exercises and problem. The last fact confirms a well-known truism: *No real learning occurs without practice.*

Exercises are essential part of this book. They are carefully selected to help readers get better understanding of the material and they are also fully solved. The difficulty of the exercises varies from simple to quite challenging.

This book *is not a standard textbook*. It differs from many excellent introductions into Quantum Physics in that it lacks the breadth and rigor

of the latter. However, this book serves a special purpose: It tries to act as the *bridge* between elementary and popular books and the more challenging college-level textbooks.

If a picture is worth a thousand words, then a formula is worth a couple of hundred words. This book contains pictures and formulas aplenty. Hopefully, the readers for whom this book is intended will enjoy both.

Some sections are marked with an asterisk, for example **Transposition***. Those sections contain material that is either optional or a bit more advanced that usual. These sections can be skipped without significant impact on the main message of the book.

At Any Cost

The subtitle of this book has been inspired by the letter from Max Karl Ernst Ludwig Planck to an American physicist Robert Williams Wood. Describing his desperate attempts to explain the experimental results on the electromagnetic radiation from hot materials, Max Planck wrote[1] (italics are mine):

> ***Max Planck to Robert Wood***
> A theoretical interpretation therefore had to be found *at any cost*, no matter how high. It was clear to me that classical physics could offer no solution to this problem, and would have meant that all energy would eventually transfer from matter to radiation. ...This approach was opened to me by maintaining the two laws of thermodynamics. The two laws, it seems to me, must be upheld under all circumstances. For the rest, I was ready to sacrifice every one of my previous convictions about physical laws. ...[One] finds that the continuous loss of energy into radiation can be prevented by assuming that energy is forced at the outset to remain together in certain quanta. This was purely a formal assumption and I really did not give it much thought except that *no matter what the cost, I must bring about a positive result.*

Trying to provide a theoretical explanation at any cost, Max Planck introduced the idea of energy quanta, initiating the development of quantum ideas and becoming "the father of quantum physics."

[1] Source!

1. Introduction

This quantum business is so incredibly important and difficult that everyone should busy himself with it.

A. Einstein in a letter to his friend Jakob Laub in 1908, as quoted by A. Wheeler in "The Mystery and The Message Of The Quantum"

Abstract In this chapter.

Quantum physics is a century-old branch of physics. Its success is unparalleled and yet quantum physics is unfinished in one sense: There is no clear and widely adopted consensus on what some of quantum ideas "really mean."

1.1 What Is Quantum Physics?

There are many characterizations of quantum physics. In essence, quantum physics is the part of physics which focuses on *quantum systems* – physical systems showing *quantum behavior*. So, what effects or phenomena are quantum?

1.2 Brief Historical Context

The year 1900 is usually considered the birth year of quantum physics. On December 14 of 1900, at the meeting ????, the German physicist Max Karl Ernst Ludwig Planck presented his theoretical explanation of the *spectrum* of electromagnetic radiation emitted by hot bodies. In his work he introduced what is now known as *Planck's constant* h, which has a physical meaning of *elementary quantum of action*.

> ***Niels Bohr On*** h
> The Danish physicist Niels Bohr, one of the founders of quantum physics, wrote:
> *"A new epoch in physical science was inaugurated, however, by Planck's discovery of the elementary quantum of action, which revealed a feature of wholeness inherent in atomic processes, going far beyond the ancient idea of the limited divisibility of matter."*
> (Atomics Physics and Human Knowledge, Quantum Physics and Philosopy, Complimentarity and Causality.)

Let's take a look at what happened before and after Planck's discovery.

Pre-History: Spectroscopy and Molecular Theory

The evolution of physics in the century preceding quantum era is fascinating. It is important to know some of pre-history in order to appreciate the context in which quantum physics was born. We will highlight two big advancements, one in experimental, and the other in theoretical departments.

Spectroscopy

First, the methods of *spectroscopy*–study of energy distribution across various wavelengths of visible and invisible light–experienced significant development. Already in 1802 an English chemist and physicist William Hyde Wollaston observed that[1] "If a beam of day-light be admitted into a dark room by a crevice 1/20 of inch broad[2], and received by the eye at the distance of 10 or 12 feet[3], through a prism of flint glass" one can see four colors (red, yellowish green, blue, and violet) separated by *dark lines*. Soon many more dark lines in the optical spectrum of the Sun were discovered and systematically studied by a German physicist Joseph Ritter von Fraunhofer. Today these *Fraunhofer lines* are understood to result from the *absorption* of radiation by different atoms in the atmospheres of the Sun and earth.

The energy absorbed by a substance can be *emitted*. The study of *emission spectra* from various bodies revealed a great deal of complexity and provided a lot of information about bodies' material composition

[1] Wollaston William Hyde 1802 XII. *A method of examining refractive and dispersive powers, by prismatic reflection*, Phil. Trans. R. Soc. **92**: 365–380

[2] 1/20 in = 1.27 mm.

[3] 10-12 feet = 3-3.7 m.

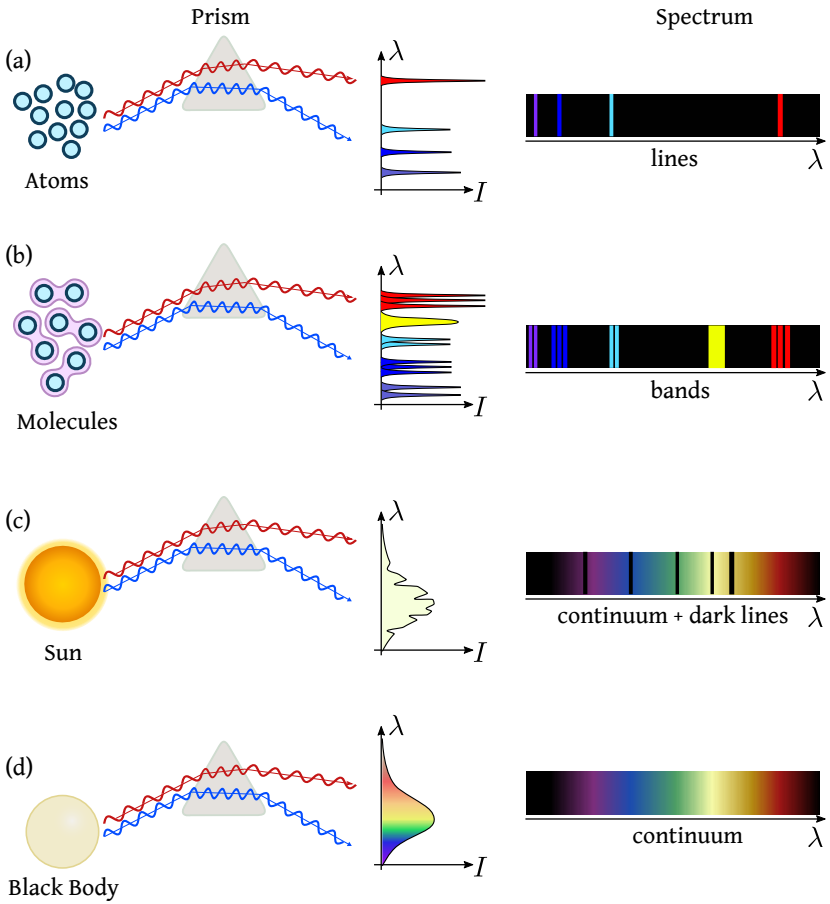

Fig. 1.1: Various types of spectra observed from different substances. (a); (b); (c); (d). See text for explanation.

and state.

There are four basic types of spectra one can observe, as illustrated in Figure 1.1. In a typical spectroscopic observation radiation from an excited object is sent through a *dispersive* component, such as a prism or a diffraction grating[4]. A beam of radiation is spread out according to colors and light of different color falls at different place of a detector (eye, photographic plate, or an electronic camera).

Light emitted by atoms consists of very definite colors which show up as *emission lines* in spectra, as shown in Figure 1.1(a). Exact locations of such lines tell which atom emits the radiation. Simpler atoms, such as hydrogen or helium, have simpler spectra.

Spectra of excited molecules contain many closely placed lines. Sometimes multiple lines coalesce into a *band*, as in Figure 1.1(b).

Radiation from large hot bodies, like Sun, reveals both discrete and continuous color distribution; see Figure 1.1(c). All colors are present in the spectrum, and dark Fraunhofer lines indicate that some of the radiation has been absorbed on its way to the detector by atoms and molecules.

Finally, an important radiation type corresponds to an *idealized* object, called *black body* – a theoretical material which does not relfect any incident radiation. In other words, *black body absorbs all incoming radiation.* Of course, black body also emits radiation, otherwise it would never stop accumulating energy from incident light. Therefore, black body *is not truly black*, its perceived color depends on the temperature of the body. Emission spectrum of black-body, called *black body radiation* or *normal spectrum*, is of great interest, because it approximates emission spectrum from *any material* kept at a constant temperature. At the end of the 19th century, black body radiation was actively studied both experimentally and theoretically.

> ***Max Planck And Black Body Radiation***
> Since black-body radiation spectrum does not depend on particular material, it has a universal nature. This fascinated Max Planck, as he wrote in his Scientific Autobiography[a]:
>
> *"Thus, this so-called Normal Spectral Energy Distribution represents something absolute, and since I had always regarded the search for the absolute as the lofties goal of all scientific activity, I eagerly set to work."*

[4] See Visual Glossary

$$\delta E = \rho \delta \nu = \frac{8\pi h \nu^3 \delta \nu}{c^3} \frac{1}{e^{h\nu/kT} - 1} .$$

[a] Max Planck, *Scientific Autobiography and Other Papers*, Williams & Norgate, 1950, pp. 34-35.

The spectrum of black body radiation was the first type of spectrum to receive a theoretical explanation and an explicit formula. Spectra of atoms and molecules were properly studied only after the development of quantum mechanics.

Spectroscopy of the 19th century[5]

Molecular Theory

Second advancement of pre-quantum physics was connected with the hypothesis of atoms and molecules. Although atomistic ideas had been known for about two millenia, even in the 19th century far from every physicist was convinced that atoms and molecules were objects just as real as everyday things. There was no *direct evidence* for the existence of atoms and molecules, and the main support for the atomistic views came from *indirect evidence*, like the many useful results that followed from molecular theory. For example, the behavior of gases (diffusion, viscosity, laws connecting pressure and temperature, heat capacity, etc.) was especially well explained. Two major figures in this field were the Scottish physicis James Clerk Maxwell and the German physicist Ludwig Boltzmann.

In September of 1899, at the congress of the German Society of Natural Scientists and Physicians, Ludwig Boltzmann presented a review titled *"The Recent Development of Method In Theoretical Physics."*[6] He highlighted the rapid development of physics in the 19th century and discussed major experimental and theoretical results.

Boltzmann's Prediction

"I have to mention finally the relations which obtain according to the molecular theory between the principle of entropy and the calculus of probabilies, concerning the real significance of which there may be some

[5] William McGucken, *Nineteenth-Century Spectroscopy*, The Johns Hopkins Press, 1969.

[6] *The Monist*, January, 1901, Vol. **11**, No. 2, pp. 226-257.

> *difference of opinion, but which, no unprejudiced person will deny, are eminently qualify to extend our intellectual horizon and to suggest new combinations both of ideas and experiments."*

Boltzmann's anticipation that "the principle of entropy and the calculus of probabilities" will lead to "new combinations both of ideas and experiments" was fully confirmed by Max Planck in about a year!

As explained in the Section XX, Max Planck used nearly the same approach as Boltzmann to calculate entropy of a thermodynamic system. Only in his case, the system was not an ideal gas of molecules, but a collection of oscillating molecules that interact with electromagnetic radiation (in the form of heat).

1.2.1 Three Ages of Quantum

The evolution of quantum science and technology can be roughly divided into three stages: (a) "Old quantum physics" (b) modern quantum physics, and (c) information-age quantum physics (see Figure 1.2).

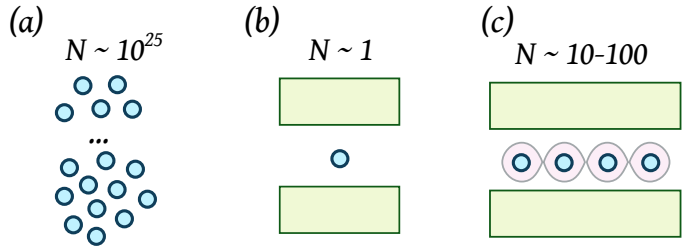

Fig. 1.2: Three stages of quantum science and technology: (a) Observation of large groups of objects (atoms, molecules); (b) Study of interaction between single particles (one atom + one photon); (c) Connecting tens and hundreds of quantum systems using *entanglement*.

Old Quantum Physics
Modern Quantum Physics
Information Age

1.3 Who Needs Quantum Physics?

In October of 1912, Albert Einstein wrote in a letter to his physicist friend Arnold Sommerfeld:

Example of mybio environment
I am now exclusively occupied with the problem of gravitation theory and hope, with the help of a local mathematician friend, to overcome all the difficulties. One thing is certain, however, that never in my life have I been quite so tormented. A great respect for mathematics has been instilled within me, the subtler aspects of which, in my stupidity, I regarded until now as a pure luxury. Against this problem [of gravitation] the original problem of the theory of relativity is child's play.

In the period from 1905 to 1916 Einstein was feverishly working on the General Theory of Relativity – the next best theory of gravity since Newton. The mathematics of general relativity is based on the calculus of tensors, created by Italian mathematicians Ricci-Curbastro and Levi-Civita roughly a decade before Einstein started working on the problem of gravity.

1.4 Why is Quantum Physics Hard?

Now what are tensors more rigorously? Can we give a short definition to this concept? Let us take a look at several examples and see whether they shed sufficient light. The definitions given below differ from each other, but they simply convey *the same idea in different ways.* sectionChallenges To illustrate the concepts of functions, operators, their structures and properties, we will be using schematics like the one

1.4.1 Mathematics

To illustrate the concepts of functions, operators, their structures and properties, we will be using

1.4.2 Language

To illustrate the concepts of functions, operators, their structures and properties, we will be using schematics like the one

The Encyclopedia of Mathematics [7] provides the following definition:

[7] `https://encyclopediaofmath.org/wiki/Tensor_on_a_vector_space`

Definition 1.1 ☞ ***Example of mydef environment***

Tensor on a vector space V over a field k is an element t of the vector space

$$T^{p,q}(V) = (\otimes^p V) \otimes (\otimes^q V^*)\,,$$

where $V^* = \mathrm{Hom}(V, k)$ is the dual space of V.

To understand this defintion we first need to understand what *vector space* is, what *field* is, what *dual* means, and what is going on with superscripts and circles (e.g., in $\otimes^q$).

1.4.3 Concepts

To illustrate the concepts of functions, operators, their structures and properties, we will be using schematics like the one

1.5 Quantum Versus Classical

Sometimes to illustrate mathematical concepts and *relations between them*, we will use diagrams. Diagrams are helpful in highlighting some general features of *mathematical structures*.

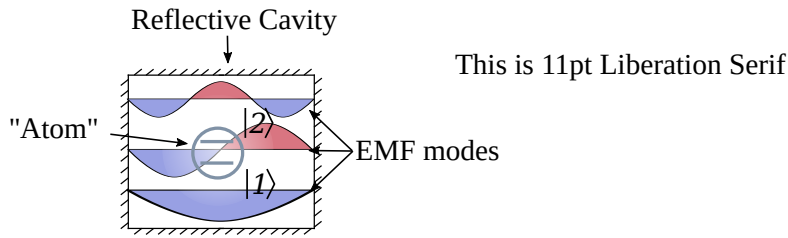

Fig. 1.3: Diagrams are used to graphically represent sets of objects and relationships between them. Arrows can connect (map) elements of one set with another. Such mappings may have names: **mlg** returns mileage for a given car, **clr** – color, and **smk** determines whether two cars are of the same make.

A particular property of a car-point can then be represented using an arrow that connects the car-point to another point in the relevant set. We say that such an arrow *maps* points of one set into another set. The Figure1.3(b) shows three maps: **mlg** gives the mileage for each car from

the set Λ, **clr** gives the color for each car, and **smk** compares whether two cars have the same make.

Exercise 1.1
Extend the diagram from the Figure 1.3(b), adding a set of different car makes (e.g., Ford, Toyota, Fiat, etc.) Come up with a mapping from this set into the Boolean set B.

1.6 Quantum Puzzle

To illustrate the concepts of functions, operators, their structures and properties, we will be using schematics like the one shown in the Figure 1.4.

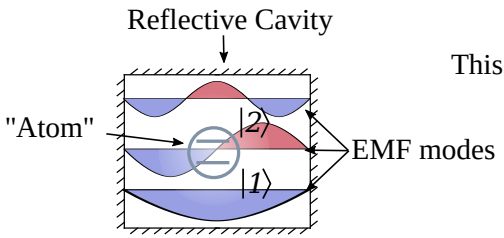

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Fig. 1.4: Schematics can be used to represent functions, operators, their compositions and structure.

A simple schematic element is represented as a box with inputs and outputs. A box can have a name (label) which describes what the function does to its input. The number of inputs and outputs can vary depending on the complexity of a function.

Chapter Highlights

- *Natural evolution of mathematical objects from numbers, through vectors, leads to tensors.*

- *Each successive tier of mathematical object in the progression "numbers, vectors, tensors" is more abstract and more powerful.*
- *Numbers, vectors, and tensors are all conceptually connected.*

2. Physics

Numbers are powerful mathematical objects. They are used to solve an endless list of problems that involve *quantities*. As mathematics and sciences progressed, natural numbers evolved into whole numbers, then into rational numbers and beyond.[1]

> ☑ ***Prerequisite Knowledge***
> To fully understand the material of this chapter, readers should be comfortable with the following concepts:
> - State
> - Dynamical equations

2.1 Goals and Methods

Physics is a *human* activity pursuing the following major goals: *Describe*, *explain*, and *predict* phenomena comprising the observed world.

results can be applied in a wide range of fields. In part, the universality of mathematics stems from the *general* and *abstract* nature of mathematical concepts. Let us illustrate this using an example.

An astute farmer notices that 49 sacks of grains can be arranged in a square with each side having 7 sacks (see the Figure 2.1). When one sack is used up, the remaining 48 sacks can be arranged as a rectangle 6 by 8 sacks.

> **Exercise 2.1** ✎
> Think how you would represent the generalized relations of the types

[1] A superb account of this process is given in the book *"Number: The Language of Science"* by Tobias Dantzig.

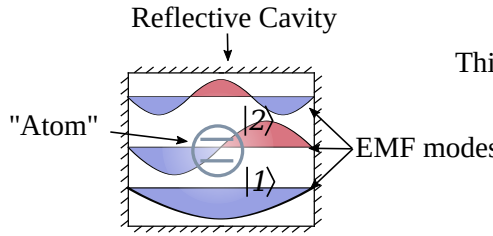


Fig. 2.1: 49 objects can be arranged in a square 7x7. 48 objects can be arranged as a rectangle of 6x8.

given in the Figure ?? at the level of sets? What kind of diagrams would you draw?

2.2 Common Sense

Mathematics is a remarkably effective and universal discipline, its methods and results can be applied in a wide range of fields.

2.2.1 Detached Observer

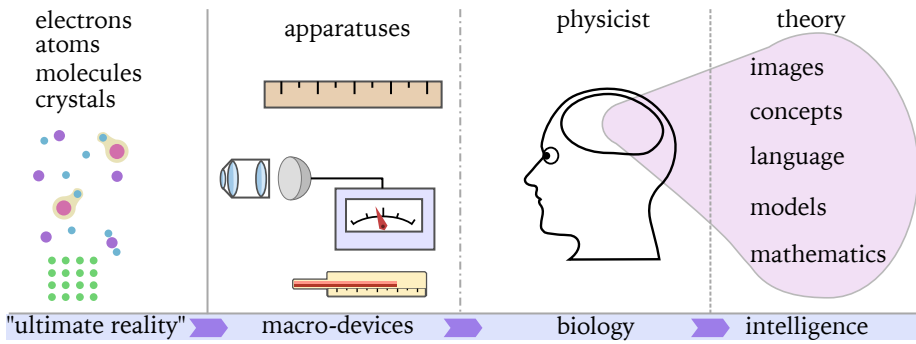


Fig. 2.2: Observers in classical view of the world are detached, separated from the "true" reality which they try to comprehend.

Object and Properties
Is it possible to separate an object from its properties?

2.3 Deterministic Evolution

The completeness of a state is a very strong constraint. Not only it means "everything there is to know at a given moment", but also "know state now – know state always." The latter is an expression of *determinism*: the complete knowledge of a system is fully determined at all times once an initial state is known. However, state by itself is not sufficient to satisfy the latter requirement, it must be supplemented by the so called *dynamical equations*. These equations are specific to a physical system and encapsulate the laws that govern internal interactions. EXAMPLE?

Denoting the mathematical representation of the state as ξ, the evolution of the state between the moments of time $T = t$ and $T = t + \Delta t$ may be written as a functional dependence:

$$\xi_{t+\Delta t} = U_{t+\Delta t,t}\, \xi_t \,.$$

For $\Delta t > 0$ we determine the future state, while for $\Delta t < 0$ we determine the state in the past (relative to the moment t).

> 💬 ***Example***
> For circular motion the state is the angle $\xi = \phi$, and the evolution is given by a simple formula
>
> $$\phi_{t+\Delta t} = U_{t+\Delta t,t}\, \phi_t = \omega \Delta t + \phi_t \,.$$
>
> Notice that in this case the evolution function depends on the time *difference* Δt and not on each moment of time separately:
>
> $$U_{t+\Delta t,t} = U_{\Delta t} \,.$$

It must be emphasized again, that the final state $\xi_f = \xi_{t+\Delta t}$ is determined by two factors: the initial state $\xi_i = \xi_t$ and the laws of physics encoded in the evolution function $U_{t+\Delta t,t}$.

$$\xi_f \xleftarrow{\quad U_{\Delta t} \quad} \xi_i$$

The laws of physics are timeless[2], as illustrated by the Coulomb's law for the force between charges q and Q at a distance r apart: $F_C = kqQ/r^2$.

[2] Technical term is *time-translation invariant.*

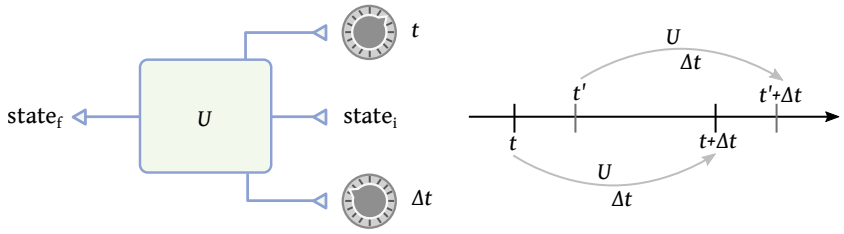


Fig. 2.3: Evolution operator transforms an initial state into the final state in time Δt.

The timeless nature of the physical laws requires that the same initial state ξ_i evolves into the same final state ξ_f regardless of when the evolution starts as long as the time interval between the beginning and the end of evolution is the same. Mathematically this is expressed as follows:

$$U_{\tau,t}\,\xi_i = U_{\tau',t'}\,\xi_i$$

for *any* initial state ξ_i, as long as $\tau' - t' = \tau - t = \Delta t$.

Thus, for *any* values of t and t', we have

$$U_{t+\Delta t,t} = U_{t'+\Delta t,t'}\,.$$

This equation says that the evolution function U becomes insensitive to the values t and t', and only depends on Δt – the time interval between the beginning and the end of evolution. Therefore, we can write the following connection between the states at different moments:

$$\xi_{t+\Delta t} = U_{\Delta t}\,\xi_t\,.$$

This connection holds *for any moment of time* t and time interval Δt.

In physics the states are represented using numbers, vectors, functions, and similar mathematical objects. Common to all of these types of objects is a very basic property of "additivity" and "scalability". That is, one can – at least formally – add and subtract states, as well as multiply them by numbers. For example, for any two states ξ_1 and ξ_2, one can write equations like

$$\xi_3 = 2\xi_1 + 3\xi_2 \qquad \text{or} \qquad \Delta\xi = \xi_2 - \xi_1\,.$$

Depending on a particular representation of the state, the evolution

function U might be a "usual" function, an operator, or something else entirely. Regardless of what the exact *type* of U is, its job is always the same – map initial state ξ_i at time t into the final state ξ_f at time $t + \Delta t$.

For $\Delta t = 0$ the evolution function U must be a simple *identity* function:

$$U_0 = I\,.$$

Furthermore, for a continuous evolution, it is necessary for small changes in time δt to produce small changes in the state $\delta\xi$:

$$\xi_{t+\delta t} = U_{\delta t}\xi_t = \xi_t + \delta\xi\,.$$

For a continuous evolution of the state, the evolution function U must be continuous. This implies that for small time intervals it produces small changes:

$$U_{\delta t} \approx I + \delta U = I + G\delta t\,,$$

where G is called the *generator* of state evolution. The meaning of the generator is clear from its definition – it specifies how fast the state evolution happens: $G = \partial_t U$.

In terms of the generator, the evolution equation can be written using the relations

$$\delta\xi = \xi_{t+\delta t} - \xi_t = \left(I + G\delta t\right)\xi_t - \xi_t = G\delta t\xi_t\,.$$

Finally, dividing both sides by δt and using the ∂-notation, we arrive at the Schrodinger-type of equation for the *continuous* state evolution:

$$\partial_t\xi = G\,\xi_t\,. \tag{2.1}$$

The equation (2.1) is a general form of state evolution equations used in physics. It appears in many cases where the dynamics of a system is described as a *continuous deterministic evolution.*

> ***Deterministic Evolution Equations***
> Equations similar to (2.1) can be found in many physical theories. In quantum theory it is Schrodinger equation, which can be written as follows:
>
> $$\partial_t|\Psi\rangle = -i\hat{H}\,|\Psi\rangle\,.$$

2.4 Classical and Quantum

Mathematics is a remarkably effective and universal discipline, its methods and results can be applied in a wide range of fields.

2.5 State

State is a very important concept in physics. It means *complete* but *minimal* knowledge about possible behavior of a given system. By *minimal*

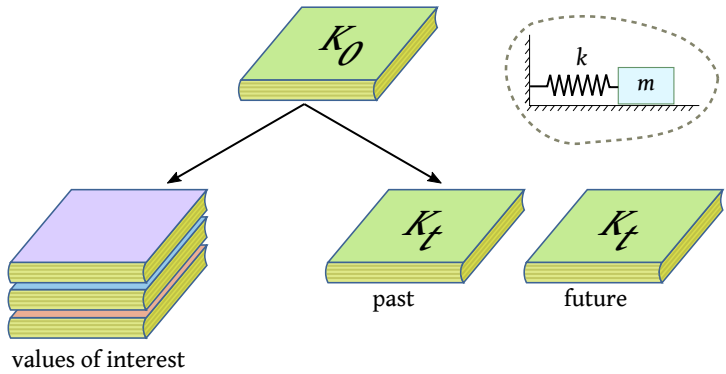


Fig. 2.4: State is a minimal and complete knowledge about a physical system.

knowledge we mean that if position of particle x is known, there is no need to know x^3 or any other one-to-one function of position. We only need to know and keep track of the *essential* information.

> ***Completeness***
> How can we be sure that the information about a system is complete? Can there be some "hidden" information, unaccessible (may be yet, or even potentially forever) to us and yet affecting the behavior of a system?
>
> The question of completeness is an important one. In the context of quantum physics it was raised for the first time by Albert Einstein, Boris Podolsky, and Nathan Rosen in 1935.

2.6 Measurement

Measurement is the source of our knowledge about the world. This is true for both classical and quantum physics.

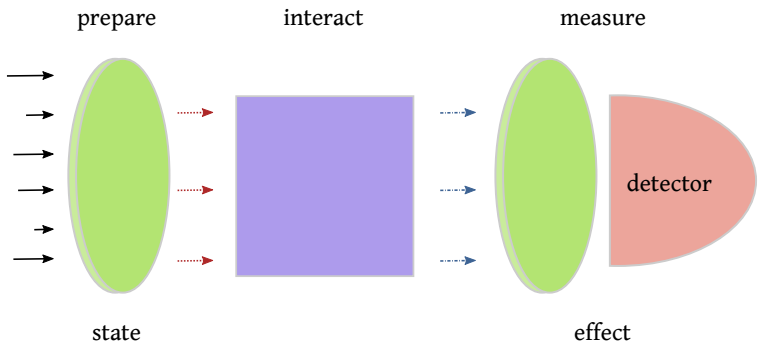


Fig. 2.5: Three stages of measurement process: Preparation of a system in a certain state, followed by the interaction of the system with external system, ending with the measurement which extract the information.

2.6.1 Joint Measurement

Imagine you put your left hand and right hand on different pads and discover that both hands move up and down randomly but in total sync.

2.7 Atoms

Classical physics predicts a continuous decay of unstable configuration of charges. What is observed is a spontaneous decay of stable configuration of charges. Quantum physics elegantly explains the latter.

2.8 Particles

Modern understanding of the particle concept is significantly more nuanced than simple "point-like object with certain physical attributes". Instead, particles are defined based on quantum behavior of corresponding *physical fields*. Quantum behavior of electromagnetic field corresponds to photons, and quantum behavior of electron-positron field corresponds to electrons (and their anti-particles).

INSERT QUOTE FROM MY SLIDES.

2.8.1 Photons And Electrons

Two types of fundamental elementary particles that will be discussed in this book are photons and electrons.

2.9 Avalanche Detectors

The dominant way humans perceive the world is through the eyesight.

2.9.1 Quantum Eyes

The first time physicists heard an effect due to a single particle (alpha-particle) was in 19xx in an experiment performed by Ernst Rutherford and Heiger.

2.10 Polarization and Spin

Mathematics is a remarkably effective and universal discipline, its methods and results can be applied in a wide range of fields.

Chapter Highlights

- *The power of mathematical concepts and methods increases with the level of abstraction.*
- *Learning new concepts often involves learning new terminology. The latter can create an artificial mental barrier.*
- *"Usual" numbers form a mathematical structure. The structure is revealed through various relations that exist between numbers.*
- *Relations between numbers are expressed using the concept of functions and operations (e.g., addition). Each operation is characterized by its arity – the number of arguments it accepts as an input.*

3. Mathematics

Mathematical concepts and tools used in quantum theory are not significantly different from the ones used in classical physics.

> ☑ ***Prerequisite Knowledge***
> To fully understand the material of this chapter, readers should be comfortable with the following concepts:
> - State
> - Dynamical equations

3.1 Functions

The idea of a function is a very basic one. Essentially, function is an unambiguous *rule*, an *algorithm*, which associates a certain value y (*result* or *output* of a function) with every meaningful *input* value x (*argument* of a function). As an example, consider the following function:

$$y = \frac{1}{2x^2 + 5}\,.$$

For any real number x we can compute the value y using only basic arithmetic operations.

Next consider a function **sqrt** which computes a square root of a number: $y = \textbf{sqrt}\, x$. If we only work with real numbers, the range of meaningful inputs is reduced – only non-negative input values x are allowed. Another thing to notice is that now the function is simply given a name **sqrt** and shows no structure – it is not expressed in terms of other more basic operations. A few important functions are given names:

$\sin$, $\cos$, $\exp$, $\log$, **abs**[1] and several more. Of course, the square root of a number is traditionally written with a special sign – called a *surd*: **sqrt** $x = \sqrt{x}$.

3.1.1 Function Boxes

The input-output view of functions leads to a helpful picture where a given function is represented as a box with an input and an output (or multiple inputs and even multiple outputs), as illustrated in Figure 3.1.

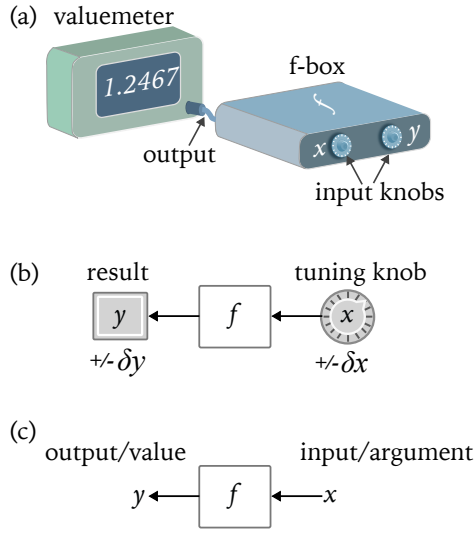


Fig. 3.1: A function can be viewed as a box with input(s) and output(s).

3.1.2 Application Notation

The dominant rule for writing function f applied to an argument x uses parentheses around the argument, like so: $f(x)$. This rule, howevers, is *not absolute* and is abandoned as soon as one uses functions in linear algebra. For example, when an operator $\widehat{f}$ is applied to a vector $|x\rangle$, we would write $\widehat{f}\ |x\rangle$, without the parentheses.

In this book we will use a uniform rule for function application: *Function and its argument are separated by a space. Only structured arguments are surrounded by parentheses. Simple arguments are written without*

[1] Absolute value of a number – its positive magnitude.

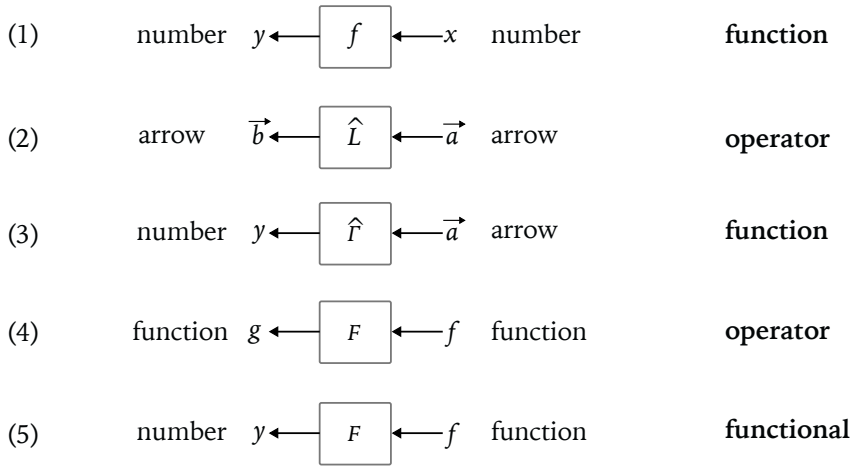


Fig. 3.2: Several types of functions: (1); (2); (3); (4); (5).

parentheses. Thus, we will always write

$$\sin x\,, \quad \exp x\,, \quad \operatorname{abs} x\,,$$

and so on. We can even write – without any confusion – expressions like

$$\cos\frac{\phi}{3}\,, \quad \log\sqrt{y}\,.$$

However, we will always use parentheses in the expressions similar to

$$\tan(\alpha+\beta)\,,$$

to avoid confusion with another valid expression: $\tan\alpha+\beta = (\tan\alpha)+\beta$.

3.1.3 Multi-Input Functions

Function of a single argument are the most familiar kind. However, functions with two inputs are also widely used. The simplest example is the function of two arguments (*binary function*):

$$\mathbf{add}\, x\, y = x + y\,.$$

On the left-hand side the function is written using so-called *prefix notation*, where the name precedes the arguments. On the right-hand side the same function is written using a more conventional *infix notation*,

in which a special symbol is placed between two arguments. Other examples if binary functions can be given:

$$\textbf{mul}\, x\, y = x * y = xy\,,$$

$$\textbf{pow}\, x\, n = x\hat{}n = x^n\,,$$

$$\textbf{max}\, x\, y = x \,\text{if}\, x > y,\ \text{otherwise}\, y\,.$$

Note that the infix notation works only for binary functions and special symbols (like "+") exist only for small number of them. In short, infix notation, although convenient, lacks generality needed for more powerful and abstract mathematics.

Any formula expressing a physical quantity can be viewed as a function with multiple inputs. Consider Newton's law for gravitational attraction between two point-like bodies. The force is given by

$$F = G\frac{Mm}{r^2}\,.$$

Assuming that the gravitational constant G is a fixed number, the expression for the force depends on three arguments – two masses and the distance between them.

Exercise 3.1
Consider a *ternary function* (function of three arguments):

$$f\, M\, m\, r = Mm/r^2\,.$$

Express it purely in terms of the binary function **mul** and the unary function **inv**.

3.1.4 Partial Application

The box-view of functions leads to a simple, yet powerful, concept of a *partially applied* function. A function of multiple arguments is called partially applied if not all its "inputs" are "filled" (i.e. assigned fixed values).

Consider, for instance, the ternary function from the Exercsie 3.1. Suppose we study how two specific bodies,with masses $M = 10$ and $m = 1$, interact gravitationally . Then the force F between these bodies

is a unary function F_r of the distance r:

$$F_r = G * (f\,10\,1\,r) = 10G/r^2\,.$$

Here we partially applied the ternary function f to only two arguments, leaving the third argument r a free parameter. As the result of such partial application we obtained a unary function of the distance r between two boides.

Let's consider another example of partial application. This illustration might seem trivial, but it will help understand the role of partial application in the case of *dual* objects, such as ket and bra vectors of quantum theory. First, we write a product of two numbers using prefix notation: **mul** $x\,y$. Then, partially apply the binary function **mul** to some number, say 3. This results in a unary function **trp** which simply triples the value of its argument:

$$f_y = \mathbf{trp}\,y = 3y\,.$$

3.1.5 Linearity

Some functions are simpler than others. For example, a *symmetric* function has the same value for x and $-x$: $f\,x = f\,(-x)$. A general function does not have such a property, and in this sense symmetric functions are simpler than a general function.

Among the simplest kinds of functions, *linear functions* are of special importance. Such functions have the following properties:

$$f\,(x+y) = (f\,x) + (f\,y) \quad \text{and} \quad f\,(ax) = a(f\,x)\,.$$

These requirements are called *linearity conditions*.

Exercise 3.2
Check whether the function **trp** is a linear function.

For numeric functions, the linearity conditions are very restricting. Linear numeric functions all have the same form:

$$f_a\,x = a * x\,,$$

for some number a. Thus, for each number a there corresponds a linear numeric function f_a and its action on any argument x is a simple multiplication by the number a.

The simuation becomes less trivial when we consider linear functions whose arguments are not simple numbers (e.g. vectors, operators, or even functions).

3.2 Numberlikes

Physics without numbers is unimaginable. But simple numbers, like *natural numbers* 1, 2, 3, and so on are very limiting. As the range of application of mathematics increased, numbers evolved from natural numbers, to *whole* numbers, to *fractions*, to *real* numbers, and then to *complex* numbers and to *quaternions*[2]. The concept of a number became increasingly less intuitive, more abstract and powerful.

Today mathematics offers several *mathematical objects* which behave essentially like numbers, but which also allow more powerful manipulations and thus can be used in wider range of problems. Examples of such *numberlikes* are *vectors*, *tensors*, and *operators*. We will explore all these objects in this chapter and will see that these three concepts are actually closely related to each other (e.g. vectors are tensors, and tensors are operators!)

Addition

The essential characteristic of numbers is the ability to *add* two of them to get another number:

$$x \boxplus y = z\,.$$

The addition operation satisfies two simple requirements

$$x \boxplus y = y \boxplus x \quad \text{– commutativity}\,,$$

and

$$(x \boxplus y) \boxplus z = x \boxplus (y \boxplus z) \quad \text{– associativity}\,.$$

Additivity is "contagious" – it propagates to other mathematical objects which operate on "usual" numbers. For example, it is easy to give a constructive meaning to the following expression:

$$f = \sin \boxplus \exp\,.$$

Here we add two numeric functions to create a new function f. To describe this function we must specify what it does to all possible arguments.

[2] Octanions are not used in physics widely enough to be discussed here.

In this case it is simply

$$f\,x = (\sin\,x) + (\exp\,x)\,.$$

Thus, the ability to add numbers leads to the ability to *add functions*. It must be emphasized, that in the expressions like $\sin \boxplus \exp$ we are not adding numerical values of the functions, we are adding functions – completely different mathematical objects. Adding functions becomes very useful for certain function types called *operators*, as explained in section 3.6.

Multiplication

Repeated addition of numbers leads to the idea of multiplication. For "normal" numbers mutiplication has two properties analogous to addition:

$$x * y = y * x \quad \text{– commutativity}\,,$$

and

$$(x * y) * z = x * (y * z) \quad \text{– associativity}\,.$$

Furthermore, mutiplication and addition possess *distributivity*:

$$x * (y + z) = x * y + x * z\,.$$

The ability to add "normal" numbers allows one to introduce *multiplication of functions*. Indeed, we can give a constructive meaning to an expression

$$f = \sin \boxtimes \exp\,.$$

It must be emphasized again: this is not a multiplication of the numeric values of the functions $\sin$ and $\exp$, it is the mutliplication of the functions themselves. To find the value of a unary function f, we simply write

$$f\,x = (\sin\,x) * (\exp\,x) = y * z\,.$$

Now on both sides of this equality we have "normal" numbers: On the left-hand side we have the value $f\,x$ of a unary function f applied to the numeric argument x, on the right-hand side we have to numeric values $y = \sin\,x$ and $z = \exp\,x$ multiplied in a "usual" way.

The example given above can be generalized to an arbitrary pair of unary numeric functions f and h. It is not difficult to convince yourself that the "product" $f \boxtimes h$ is commutative, associative, and is also

distributive with respect to the "addition":

$$f \boxtimes (h \boxplus g) = (f \boxtimes h) \boxplus (f \boxtimes g)$$

for three unary numeric functions f, h, and g. In other words, unary numeric functions can be made to behave like numbers. One can view functions and manipulate them as objects on their own, without referring to their arguments.

> ***Point-free Notation***
> Manipulating functions without explicitely writing their arguments is known as *argument-free notation* or *point-free notation*. It is a useful practice and is common in quantum theory.

Composition

Functions, and their "brothers" operators, allow an additional way to combine two function in order to create another one. It is called *composition* or, sometimes, *sequencing* of two functions. Let's illustrate the idea using the familiar functions $\sin$ and $\exp$. We can "create" (define) a function f which acts on its input argument in the following way:

$$f\, x = \sin(\exp x)\,.$$

We first apply the function $\exp$ to the input argument x to obtain a numeric value $y = \exp x$, and then apply the function $\sin$ to y. We applied two functions in sequence. A special notation exists for composition. We write $f = \sin \circ \exp$. Here is used an argument free notation, writing simply f instead of "f of x", similar how we write numbers simply as n instread of "n apples".

Unlike addition and multiplication, *composition is not commutative*:

$$\sin \circ \exp \neq \exp \circ \sin \quad \text{because} \quad \sin(\exp x) \neq \exp(\sin x)\,.$$

However, *composition is associative.* Given three functions f, h, and g we can combined them in two different orders, specified by the parentheses:

$$(f \circ h) \circ g = f \circ (h \circ g)\,.$$

Both sides of this equality represent the same value $f(h(g\,x))$: We first

evaluate $y = g\,x$, then feed it into h to find $z = h\,y$, and finally input it as the argument to f.

Exercise 3.3
Check whether composition is distributive with respect to an "addition" of functions.

Composition In Quantum Physics

Composition is an very powerful way of creating new functions by combining a given pair of functions. Composition has special significance for *linear operators* – linear functions operating on non-numeric arguments (e.g. on vectors).

In quantum theory different operators represent different measurement operations, such as measurement of position, momentum, energy, angular momentum, spin, and so on. Only *linear operators* are used in quantum theory. These operators act on special vectors, as we will later learn.

Like any two functions, two quantum operators $\widehat{A}$ and $\widehat{B}$ can be composed:

$$\widehat{C}{=}\widehat{A} \circ \widehat{B}\ .$$

It is customary to drop the infix composition sign and simply write $\widehat{C}{=}\widehat{A}\widehat{B}$.

An operator can be composed with itself. In this case a special notation exists to avoid long and clumsy expressions:

$$\widehat{A} \circ \widehat{A}{=}\widehat{A}\widehat{A}{=}\widehat{A}^2\ .$$

In general, the expression $\widehat{A}^n$ represents the operator $\widehat{A}$ composed with itself n times.

3.3 Kalcoolus

Quantum theory uses many mathematical tools.

3.3.1 $\Delta - \delta - \partial$ Notation

3.3.2 Bernouli Sums

3.4 Arrows

To arrive at the idea of vectors we will start with simple geometrical objects – arrows in a plane, as illustrated in the Figure 3.3.

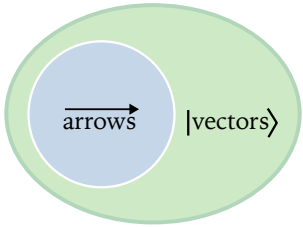


Fig. 3.3: Arrows provide a simple geometric example of vector quantities. The idea of vectors, however, is more powerful and extends beyond this simple representation as directed line segments.

Symbolically, we will denote vectors by placing an arrow over letters:

$$\vec{a}\,,\vec{b}\,,\vec{c}\,,\ldots,\vec{\alpha}\,,\vec{\beta}\,.$$

3.4.1 Dirac Notation

3.4.2 Basis and Bases

Given a basis, it become immediately apparent that it is not unique. Indeed, at least the order of basis arrows is not fixed. Also, if $\vec{e}_1$ is independent of $\vec{e}_2$, then so is $2\vec{e}_1$.

3.5 Scalar Product

To arrive at the idea of vectors we will start with simple geometrical objects – arrows in a plane, as illustrated in the Figure **??**.

3.6 Operators

To arrive at the idea of vectors we will start with simple geometrical objects – arrows in a plane.

$$\langle\phi|\phi\rangle$$

and

$$|\phi\rangle\langle\phi|\,.$$

■ **Example 3.1** Consider an operator that transforms the state $|0\rangle$ into a linear combination $|+\rangle = (|0\rangle + |1\rangle)/\sqrt{2})$ and the state $|1\rangle$ into a linear combination $|-\rangle = (|0\rangle - |1\rangle)/\sqrt{2})$.

It is called *Hadamard* operator and has the following matrix representation. ■

3.6.1 Super-operators

An action of an operator F on arrows can be represented symbolically as an equation:

$$F\,\vec{a} = \vec{b}\,.$$

Often a "hat" is placed on top of an operator[3], to emphasize that it is different from numeric function:

$$\boxed{\widehat{F}\;\vec{a} = \vec{b}\,.}$$

Simple Operators

It is easy to come up with examples of operators:

- Unit operator (or *identity* operator), such that

$$\widehat{I}\;\vec{a} = \vec{a}\,.$$

- "Zeroing" operator that maps every vector into a zero vector:

$$\widehat{0}\;\vec{a} = \vec{0}\,.$$

To fully describe an operator, we must describe how it acts *on every* arrow.

Examples

Let us take a closer look at a couple of operators. While studying these examples we must keep in mind that the relations between components are *specific to basis* and will change if we change the basis. The question of

[3] In Quantum Mechanics, for example.

how exactly the relation between components changes will be addressed later in Section **??** for the simplest types of operators.

Matrix

Here is an example of matrix:

$$\widehat{S} = \begin{pmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{pmatrix} = \begin{pmatrix} \alpha & 0 \\ 0 & \alpha \end{pmatrix}.$$

Similar approach can be used to find the components of any linear operator.

3.7 Functionals

Another important type of function is called *functional*. A functional maps a function into a number. Let's consider several examples.

Total Mass

Suppose an astrophysicist is trying to model a spherically symmetric star and calculates *density* of the star as the function of distance from its center: $r \to \rho_r$. The total mass of the star can then be evaluated as the sum of masses of all spherical shells with thickness δr:

$$M = \int \delta V \rho_r = \int 4\pi r^2 \delta r \rho_r \,.$$

For a given function ρ_r this summation will result in a number – star's total mass. Such mapping $\rho_r \to M$ is an example of a functional.

Total Fuel

Consider a car moving on a straight highway between two points A and B. The amount of fuel the engine consumes at a given moment depends on the speed of the car at that moment and can be described by the function μ_v. Suppose the position of the car as the function of time x_t is known and are looking for the total fuel consumed during the travel. This can be done in three steps.

First, we find the speed of the car as the function of time by applying the operator ∂_t to x_t: $v_t = \partial_t x$. Second, we find the fuel consuption rate

μ as the function of time by plugging v_t into μ_v: $f_t = \mu(v_t)$. Finally, we can find the total amount of consumed fuel as the sum

$$F = \int f_t \delta t \,.$$

Combining all three steps into a single mathematical expression will result in a more cumbersome formula:

$$F = \int \delta t \mu(\partial_t x) \,.$$

This formula encodes a recipe for mapping any function x_t into a number F – an example of a functional.

Total Action

A body in a "free fall" is moving with constant acceleration due to the force of gravity. Its speed increases as the body approaches the ground. If the body starts at rest at height H, its position along the vertical y axis depends on time as $y_t = H - gt^2/2$ and the velocity changes according to the equation $v = -gt$.

The potenital energy $E_p = mgy$ of the body decreases, while its kinetic energy $E_k = mv^2/2$ grows. The total mechanical energy $E = E_p + E_k$ remains fixed according to the law of energy conservation. Thus, the potential energy of the body is transformed into the kinetic energy.

Another physical quantity is often important – the *imbalance* of kinetic energy over the potential energy:

$$L = E_k - E_p \,.$$

It does not remain constant, and for the case of a free fall we can easily find its time dependence:

$$L_t = mg^2t^2 - mgH \,.$$

Given L_t, we can calculate a fundamental physical quantity – total *action* of the process:

$$A = \int \delta t L_t \,.$$

The summation extends to the moment $t = T$ when the body reaches the ground ($y = 0$). This happens at $T = \sqrt{2H/g}$.

Performing the summation requires evaluation of two familiar sums:

$$\int t^2 \delta t = \frac{T^3}{3} \quad \text{and} \quad \int \delta t = T\,.$$

Substituting the values of T and simplifying, the expression for the total action takes the form

$$A = mgT\left(\frac{gT^2}{3} - H\right) = -\frac{mH}{3}\sqrt{2gH} = -\frac{mv_m H}{3}\,.$$

Here we used $v_m = gT = \sqrt{2Hg}$ – the maximal speed of the body at the end of the free fall process. Finally, denoting the maximum momentum of the body as $p_m = mv_m$, we obtain $A = -p_m H/3$. Note that the action can be expressed as the product of momentum and distance.

Action is a physical quantit of fundamental importance. It plays a prominent role in both classical mechanics (the principle of *stationary action*) and in quantum physics (the principle of *action quantization*). Both principles will be explored in details later in the book.

Exercise 3.4
Calculate the total action of a free fall process for an electron falling from the height 0.1 meter.

Assorted Examples

Examples of functionals given above involve evaluation of sums in order to find *total quantities* of various kinds:

$$Q = \int \delta x f_x\,.$$

The total quantity Q depends on the behavior of the input function f_x over an extended range of x values. Simpler forms of functionals can also be used. For example:

$$\mathcal{M} f = f_0$$

returns the value of the input function f_x at zero. This functional, despite its trivial look, is very useful and widely used in physics and mathematics. Its rigorous mathematical form is called *Dirac delta function*.

Dirac Delta Function

The idea of delta function is simple: it describes the density of mass (or charge, probability, and so on) for a point-like particle. Formally, such density can be written as δ_x.

Since the total mass (charge, probability) is finite, the summation of the density over the region where the particle might be must be a fixed number:

$$m = \int \delta x \delta_x \, .$$

Another example of a simple functional is the maximum of a function:

$$\mathcal{X} \, f = \max f_x \, .$$

Finally, one can map any function f_x into a number like so:

$$\mathcal{R} \, f = \frac{f_1}{1!} + \frac{f_{1/2}}{2!} + \frac{f_{1/3}}{3!} + \ldots + \frac{f_{1/n}}{n!} + \ldots \, .$$

For $f = \sin$ we obtain $\mathcal{R} \sin \approx 1.1479$.

Exercise 3.5

For the functionals $\mathcal{M}$, $\mathcal{X}$, and $\mathcal{R}$ check whether they are *linear*.

3.8 Spaces

To arrive at the idea of vectors we will start with simple geometrical objects – arrows in a plane.

$$\langle \phi | \phi \rangle$$

and

$$|\phi\rangle\langle\phi| \, .$$

3.9 Duality

To arrive at the idea of vectors we will start with simple geometrical objects – arrows in a plane.

$$\langle \phi | \phi \rangle$$

and

$$|\phi\rangle\langle\phi| \, .$$

3.10 Bundling

A pair of vectors can be combined in a variety of ways. For example, adding two vectors returns the third vector, while scalar product returns a number. Other useful methods of combining vectors result in more advanced mathematical objects, such as, for example, tensors. One simple approach to combining vectors to create complex objects uses the idea of *bundling*.

When a pair of vectors is bundled, the original vectors are not lost, they become incorporated in a more complex mathematical object. It may sound complicated, but the idea can be expressed simply as follows: *Keep original vectors together in some some sort of a bundle.*

The simpest bundle is a pair. Given two vectors of the same type $|a\rangle$ and $|b\rangle$ we can bundle them into a pair: $\mathcal{P} = (|a\rangle, |b\rangle)$.

$$|a\rangle\langle b|\,.$$

Exercise 3.6

Write Hadamard operator in terms of the tensor product of vectors $|0\rangle$, $|1\rangle$, $|+\rangle$ and $|-\rangle$.

$$\widehat{H} = |+\rangle\langle 0| + |-\rangle\langle 1|\,.$$

3.11 Functions As Vectors

To arrive at the idea of vectors we will start with simple geometrical objects – arrows in a plane.

$$\langle\phi|\phi\rangle$$

and

$$|\phi\rangle\langle\phi|\,.$$

3.12 Application: Circular Motion

Let us examine how the concepts and tools discussed above can be applied to a simple case of circular motion.

Consider a particle moving in a circle with the radius R, as shown in Figure X. If we choose the center of the circle as the reference point,

we can specify the position of the particle using an arrow $|r\rangle$. During motion the direction of this arrow is constantly changing, but its length R remains the same.

After a short time interval δt, the position of the particle changes by $\delta|r\rangle$:

$$|r_t\rangle \quad \rightarrow \quad |r_{t+\delta t}\rangle = |r_t\rangle + \delta|r\rangle\,.$$

The length of the path covered by the particle during the time interval δt can be approximated by the length of the arc $\delta L = R\delta\theta = v\delta t$. The arrow $\delta|r\rangle$ can be written as $\delta L|u\rangle$ where $|u\rangle$ is the vector of unit length pointing in the direction of motion. This unit vector can be constructed from $|r\rangle$ by scaling it down by R and then rotating counter-clockwise with the operator $\widehat{J}$:

$$\delta|r\rangle = R\delta\theta\ \widehat{J}\left(\frac{|r\rangle}{R}\right).$$

Since $\widehat{J}$ is a linear operator, the R cancels and we can write

$$\frac{\delta|r\rangle}{\delta t} = \frac{\delta\theta}{\delta t}\ \widehat{J}\,|r\rangle \qquad \Longrightarrow \qquad \partial_t|r\rangle = \omega\ \widehat{J}\,|r\rangle\,,$$

where we introduced the angular speed $\omega = \partial_t\theta$. Finally, by applying the $\widehat{J}$ operator to both sides of the last equation, we can cast it into the "Schrodinger" form:

$$\widehat{J}\ \partial_t|r\rangle = -\omega|r\rangle\,.$$

Chapter Highlights

- *Arrows in a plane provide a simple model for vectors.*
- *Arrows can be manipulated in ways analogous to numbers: Two arrows be added, an arrow can be "scaled" (stretched or compressed). Arrows form an algebra.*
- *Basis is an extremely important concept. Basis is a set of objects (arrows) that can be used to "build" all other similar objects (arrows). At the same time, basis can not be used to build itself – basis arrows are independent.*

4. Classical Physics

> *I think we may ultimately reach the stage when it is possible to set up quantum theory without any reference to classical theory, just as we already have reached the stage where we can set up the Einstein gravitational theory without any reference to the Newtonian theory. But from the point of view of teaching students, I think one would always have to proceed by stages – not expect too much from them, teach them first the elementary theories and gradually develop their minds; and that will always involve working from the classical theory first.*
>
> *P. A. M. Dirac, Lectures on Quantum Field Theory, Belfer Graduate School of Science, Yeshiva University, New York, 1966, p.43.*

The concept of *operators* extends the idea of functions. An unary numeric function f takes some numeric value x as an input and produces another numeric value y:

$$f\,x = y \quad \text{or} \quad x \xrightarrow{f} y\,.$$

In mathematical jargon, f *maps* x into y.

☑ ***Prerequisite Knowledge***

To fully understand the material of this chapter, readers should be comfortable with the following concepts:

- State
- Dynamical equations

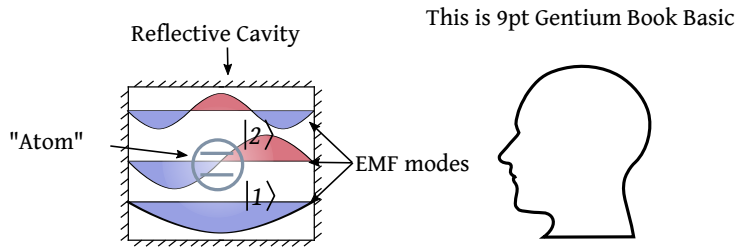


Fig. 4.1: Operators extend the idea of functions. (a) An unary function f can be applied to a number x to produce another number y. (b) An unary operator $\widehat{F}$ can be applied to a vector $\vec{a}$ to yield another vector $\vec{b}$.

4.1 System

A part of nature that can be clearly isolated and studied is called a *physical system*. An electron, an atom, a molecule, a crystal, a pendulum, a comet, a star – these are examples of physical systems of various degrees of complexity.

Often a physical system is a body or several bodies interacting with each other or with some external bodies. Figure 4.2 provides several examples of *mechanical systems*. Let's examine them in more detail.

(a) *Free falling body*: An elastic body falls down vertically under the force of gravity, bounces back, goes up and then down to repeat the bounce again and again. Also, a projectile launched at an angle.
(b) *String pendulum*: A compact body is attached to a string of fixed length. It is allowed to swing back and forth without experiencing air friction.
(c) *Atwood machine*: Two bodies with slightly unequal masses are connected with a non-stretchable string going over a frictionless pulley.
(d) *Inclined plane*: A solid cylinder rolling down an inclinded plane.
(e) *Piston*: A system of three bodies (cylindrical crankshaft, rod, and piston) connected in a way that locks rotation of a cylinder and the vertical motion of the piston.
(f) *Spring oscillator*: A body, attached to a spring, is allowed to slide left and right across a frictionless surface.
(g) *Linear chain of oscillators*: A set of pairwise interconnected iden-

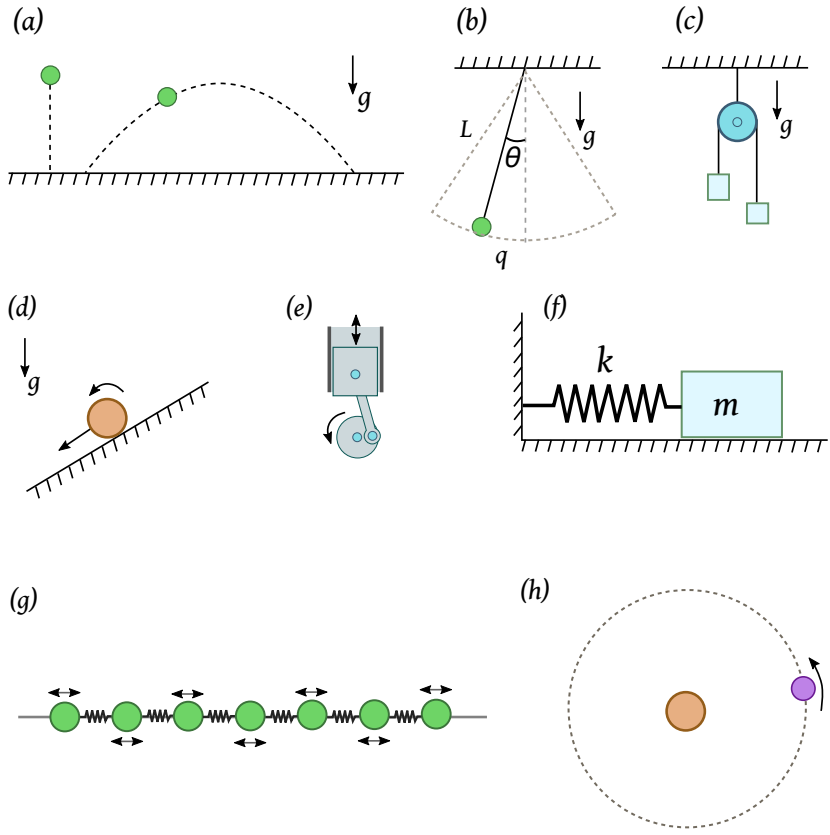


Fig. 4.2: Examples of mechanical systems. See text for explanation..

tical bodies; the allowed motion happens along the horizontal axis.

(h) *Sun and planet*: A planet circling around the sun.

We will study oscillator and circular motion in great detail.

4.1.1 Configuration

In mechanics, *configuration* means a formal way to describe the arrangement of a system at a given time.

The behavior of a system in time can be described by specifying its *configuration* as the function of time. In relatively simple systems, configuration may consist of a set of coordinates that uniquely determine the arrangement of bodies in the system. For example, the configuration of a pendulum can be given by a single coordinate — the length of the arc q. Of course, as the pendulum swings, both Cartesian coordinates x and y are changing, but not independently, due to the relation

$$x^2 + y^2 = L^2 \,.$$

Given x, we can find $y > 0$ as $y = +\sqrt{L^2 - x^2}$, thus reducing the number of required coordinates.

Consider another example, shown in the Figure (4.3)(a): a system of two bodies, connected with each other using ideal springs with stiffness k, and each body is connected to a rigid wall.

When the system is in equilibrium, the bodies occupy positions on the horizotal axis denoted as e_1 and e_2. During motion, the position of the first body changes by

$$q_1(t) = x_1(t) - e_1 \,,$$

and similarly for the second body: $q_2 = x_2 - e_2$. It is important to realize, that although the two bodies are connected with a spring, they can still move with different velocities, and have different displacements $q_1 \neq q_2$. Indeed, we can set the system in motion by moving each body independently and then releasing them. Contrast this with the situation, shown in the Figure (4.3)(b), where the bodies are connected with a rigid rod, fusing two masses into essentially a single body. In this case only a single displacement q is required to specify the configuration of the system.

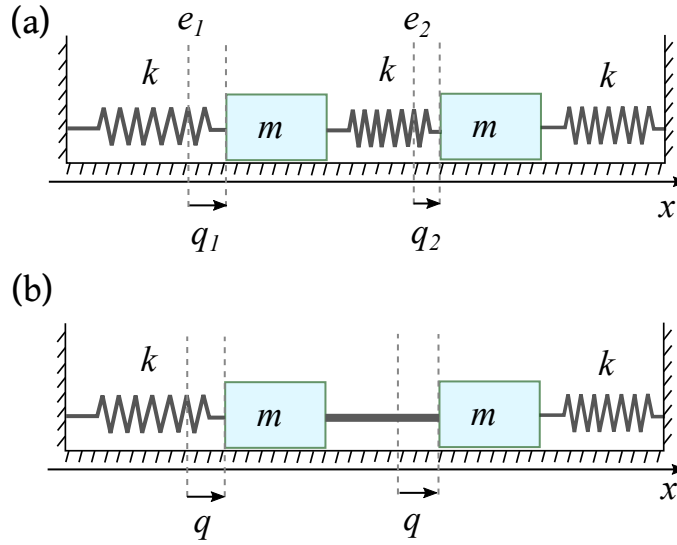


Fig. 4.3: (a); (b).

4.1.2 Qoordinates

The coordinates specifying the configuration of a system do not have to be Cartesian. In the example of a pendulum, the configuration can be conveniently given by the length of the arc $q = L\theta$, see Figure (4.2)(b).

Consider another example, shown in the Figure (4.2)(h): Two bodies interact gravitationally. In this problem, it turns out, the equations describing the motion of the system are simpler if, instead of the usual positions x_1 and x_2 we use the relative distance

$$q_1 = x_2 - x_1$$

and the position of the center of mass

$$q_2 = (m_1 x_1 + m_2 x_2)/(m_1 + m_2),$$

where m_1 and m_2 are the masses of the bodies.

We thus come to the idea of *generalized coordinates* – arbitrary coordinates completely specifying the configuration of a system. Generalized coordinates can be based on positions, angles, or some combinations of those.

4.1.3 Degrees of Freedom

Degree of freedom is a separate independent motion of a mechanical system. Each independent motion corresponds to the change in time of a separate generalized coordinate. The number of degrees of freedom is the number of generalized coordinates required to completely specify the configuration of a mechanical system at different moments of time.

Take, for example, a pendulum, shown in the Figure (4.4). In general Cartesian coordinates, all three coordinates x, y, and z will be changing in time. However, only a single generalized coordinate $q(t)$ — the length of the arc – is required to fully describe the configuration, and thus the motion, of this mechanical system. The number of degrees of freedom, in this example, equals 1.

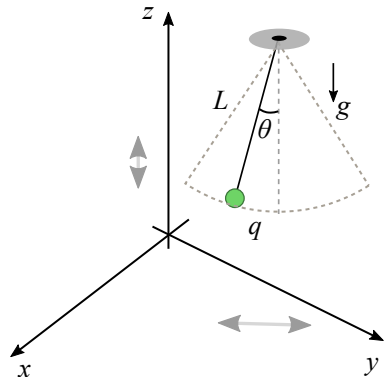


Fig. 4.4: A pendulum has one degree of freedom, despite the fact that all three Cartesian coordinates can be changing during its motion.

4.2 Oscillator

The model of an oscillator is extremely important. It appears in various guises in almost all physical theories. Let's study it in details.

Consider a body with the mass m is attached to a spring with the stiffness k. The body is allowed to move across a frictionless surface. The force required to strech a spring by the amount x is given by the Hooke's law

$$F = kx.$$

This is the force applied *to the spring*. The force created *by the spring, and applied to the attached body*, is of equal magnitude but points in the

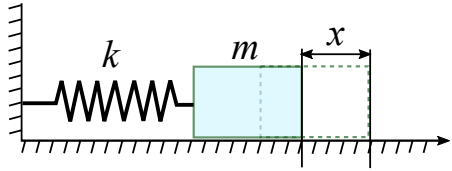


Fig. 4.5: A mechanical model of an oscillator: A body attached to an ideal spring.

opposite direction.

When the body is displaced from its equilibrium position, by stretching or compressing the spring, and then released, it will undergo periodic motion. During this motion, the position, velocity, kinetic energy of the mody, and the potential energy of the spring will be constantly changing.

To remind, the kinetic energy of a body is

$$E_k = \frac{mv^2}{2}, \text{ or } K = \frac{p^2}{2m}.$$

The potential energy of a spring, stretched or compressed by the amount x is given by

$$E_p = \frac{kx^2}{2}, \text{ or } \Pi = \frac{kq^2}{2}.$$

4.3 State

State of a system is the *minimal* collection of observables which is, in certain sense, *complete* and *self-sufficient*. State is "all there is to know" about a system. If the state of a system is known at one moment of time t_0, then we should be able to determine the state at any later moment of time t. In classical mechanics the pair of observables (x, p) defines the state of a mechanical system.

State is the minimal set of quantities describing mechanical system and sufficient to predict their future values from their initial values. State is an important concept not only mechanics, but in other areas of physics. Let's elaborate, using the oscillator as an example.

Suppose that at the moment of time t_0 the position of an oscillator is x_0 and its velocity is v_0. To find their values at some later time $t > t_0$, we can go iteratively in small steps, calculating how much the position and the velocity change after each successive tiny interval of time δt. The

first iteration results in the updated value of position

$$x_1 = x_0 + v_0 \delta t.$$

The second, and every other, iteration looks very similar:

$$x_2 = x_1 + v \delta t\,.$$

Now it is important to realize that we can no longer use the same initial velocity v_0 in the second iteration, because the velocity itself changes. Thus, we must update the value of the velocity as well. This is done by using acceleration:

$$v_1 = v_0 + a_0\,.$$

After that, we can find the second iteration of the position: $x_2 = x_1 + v_1 \delta t$. To keep this scheme going, we must be able to update the value of the acceleration, because it is also changing. It appears then, we need some quantity that allows to find the next step:

$$a_1 = a_0 + b_0 \delta t\,.$$

Fortunately, *this is not needed!* At this point we can use the laws of motion. For example, Newton's second law gives the acceleration in terms of the known force acting on the object:

$$a = \frac{F}{m}. \tag{4.1}$$

Forces don't depend on acceleration. (Weber Electrodynamics?)

All known forces in physics depend on positions or distances and– sometimes– velocities of bodies. For example, the force of the spring $F = -kx$ depends only on the coordinate x. The force of gravitational interaction $F = GMm/r^2$ and the Coulomb force between two charges $F = kQq/r^2$ depend on the distance r between the bodies. The force acting on an electron moving through a magnetic field–known as Lorentz force– equals $F = qvB$ and depends on the electron's velocity (and the field's strength B). No known forces depend on acceleration. This fact leads to an important conclusion: It is enough to know position and

velocity of an object at time t_0, in order to find their values at any later moment of time $t > t_0$. Obviously, position and velocity at any previous moment of time can be found in the similar way.

Thus, we do not need to advance the acceleration by calculating its small change $\delta a = b\delta t$, we can simply calculate it from the law of motion:

$$a_n = \frac{F(x_n, v_n)}{m} . \tag{4.2}$$

This formula says that the acceleration at the iteration step number n is found from the values of the position x_n and the velocity v_n at the same step. Given the velocity, we can advance the postion, and given the acceleration, we can advance the velocity. Then we recalculate the new value for the acceleration and repeat, until we reach the final time t.

The preceding discussion demonstrates that in Newtonian mechanics *the state of a mechanical system* is given by a pair of quantities – (x, v). There are alternatives to the Newtonian mechanics, and, correspondingly, there are alternatives to the mechanical state. The first such alternative is Hamiltonian dynamics.

4.3.1 State Evolution: Newtonian Approach

We will now apply the ideas and formulas of Newtonian mechanics to an oscillator. We will calculate the motion of the oscillator in time using a simple method of *state evolution*. Specifically, we will setup two simple equations – one for position and one for velocity.

The equation for position is trivial and amounts to the definition:

$$\frac{\delta x}{\delta t} = v .$$

The equation for velocity follows from the second law of Newtonian dynamics:

$$\frac{\delta v}{\delta t} = \frac{F}{m} = -\frac{kx}{m} .$$

Here we used the expression for the spring force $F = -kx$ acting *on the body* from the side of the spring.

Suppose we know the *initial state* of the oscillator (x_0, v_0) at time $t_0 = 0$. When the clock makes a single tick after a tiny time interval δt the body will move to a new position

$$x_1 = x_0 + v_0\delta t$$

and the velocity will change due to the action of the spring:

$$v_1 = v_0 - \frac{kx_0}{m} .$$

Thus, after a single tick of the clock the state of the oscillator will evolve from $|\xi\rangle_0 = (x_0, v_0)$ to $|\xi\rangle_1 = (x_1, v_1)$. At this point we can keep repeating the steps to calculate the state after any number of ticks, up to the desired time $t = N\delta t$.

We can now formalize the recipe for evolution of the state, writing it as a mathematical relation:

$$|\xi\rangle_{new} = f\,|\xi\rangle_{old} ,$$

where

$$|\xi\rangle_{new} = (x_{new}, v_{new}) = (x_{old} + v_{old}\delta t, v_{old} - kx_{old}/m) .$$

Using this simple approach, we can calculate the state $|\xi\rangle = (x, v)$ of the oscillator for any moment in the future or past. Figure 4.6 shows two example results. The first result, in the column (a), demonstrates that we must be careful with the step size δt of the time. If it is not sufficiently small, the inherent error of the method accumulates quickly, resulting in wrong behavior, such as the gradual increase of velocity and oscillation amplitude. The column (b) of Figure 4.6 demonstrates the expected behavior of the oscillator – periodic change of position and velocity with constant amplitudes.

4.4 Dynamics

Dynamics is the study of state evolution of various systems subject to known interactions. Physical systems of interest can be mechanical, like the ones given in example above (WHERE? REF), or "non-mechanical" like electromagnetic field or even gravitational field. One can also explore dynamics of quantum systems.

The central equation in dynamics describes the state change in time due to known *laws of dynamics*:

$$\partial_t\,|\xi\rangle = \widehat{D}_{int}\;|\xi\rangle .$$

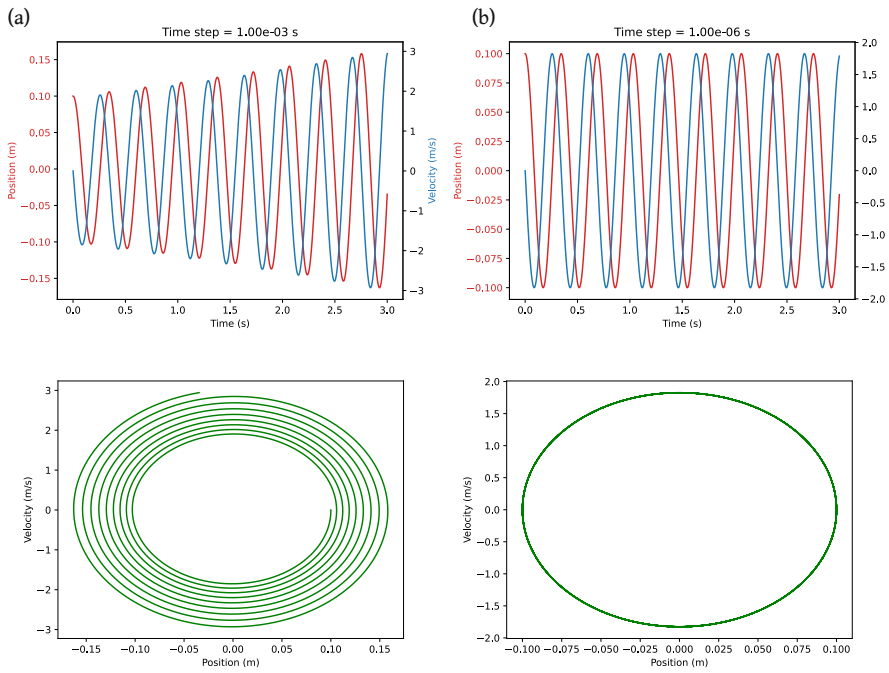


Fig. 4.6: First row: Position (red curve, left axis) and velocity (blue curve, right axis) as functions of time. Second row: Velocity vs position. (a) Calculations with time step of 1 millisecond. (b) Calculations with time step of 1 microsecond.

We will explore three main variants of classical dynamics: Newtonian, Hamiltonian, and Lagrangian. They will prepare us for better understanding *quantum dynamics*.

Newtonian dynamics is based on the notion of *force* as the driver of interaction:

$$(\partial_t x,\, \partial_t v) = (v, F/m)\,.$$

Both Hamiltonian and Lagrangian mechanics rely on the notion of energy.

4.5 Hamiltonian

Hamiltonian is the expression for total energy of a system in terms of position and momentum. For example, using the non-relativistic expression for momentum $p = mv$, the Hamiltonian of an oscillator can be written as

$$H = \frac{p^2}{2m} + \frac{kx^2}{2}\,. \tag{4.3}$$

Hamiltonian, denoted simply as H, still means the total energy. The only difference between H and E is the emphasis on the use of momentum in H instead of velocity.

Momentum is more fundamental than velocity.

Although velocity feels more intuitive and closer related to our visual perception of motion, momentum is a more *fundamental quantity* in physics. There is a *conservation of energy and momentum* law, but there is no law of the conservation of velocity.

4.5.1 Phase Space

Hamiltonian dynamics uses position x and momentum p to study motion. For an isolated system with conserved energy (constant Hamiltonian), the expression for the Hamiltonian establishes the relationship between x and p for all moments of time. For example, using the Hamiltonian for an oscillator (4.3), we can rewrite it as follows:

$$1 = \frac{p^2}{(2mH)} + \frac{x^2}{(2H/k)}\,. \tag{4.4}$$

This has the same form as the equation of an ellipse in Cartesian axes (x, y):

$$1 = \frac{y^2}{b^2} + \frac{x^2}{a^2}\,.$$

The area of such an ellipse with the semi-axes a and b is $A = \pi ab$. For $a = b$ an ellipse becomes a circle with the area $A = \pi R^2$.

The equation (4.4) describes an ellipse in a special xp-plane, every point of which can be specified by a pair of values (x, p). Such a plane is called *phase space*. It plays an important role in Hamiltonian dynamics.

The maximum value of the momentum is $p_{max} = \sqrt{2mH}$ and the maximum value for the displacement of the body is $x_{max} = \sqrt{2H/k}$. It turns out, the *area of the ellipse in the phase space is directly proportional to the total energy of the oscillator*:

$$A = \pi x_{max} p_{max} = 2\pi H\sqrt{m/k}\,,$$

or

$$H = \frac{A}{2\pi}\sqrt{\frac{k}{m}}\,.$$

This important relationship will be used later when we will study quantum properties of the oscillator.

4.5.2 Hamiltonian Equations

Hamiltonian dynamics tracks the time dependence of position x_t and momentum p_t. The pair of values (x, p) represents the *state in Hamiltonian dynamics*. Indeed, since there is a unique relationship between the momentum and velocity (e.g. $p = mv$ for non-relativistic speeds $v \ll c$, c — speed of light), the knowledge of $|\xi\rangle = (x, p)$ is equivalent to the knowledge of $|\xi\rangle = (x, v)$ which is the state in Newtonian dynamics. Put differently, the pair (x, p) provides the same complete description of the system as (x, v).

The main difference between Newtonian and Hamiltonian approaches, is that in the latter the equations for the rate of change of x and p are *explicitly tied to the Hamiltonian*— to the form of the energy expressed in terms of position and momentum. In other words, the equations for $\partial_t x$ and $\partial_t p$ are written in the following form:

$$\partial_t x = \widehat{X}\ H \qquad \text{and} \qquad \partial_t p = \widehat{P}\ H\,.$$

where $\widehat{X}$ and $\widehat{P}$ are some *rules* for calculating velocity $v = \partial_t x$ and force $F = \partial_t p$ from Hamiltonian H. Mathematically, $\widehat{X}$ and $\widehat{P}$ must be *operators*: they take the function $H(x,p)$ and calculate the functions $v(x,p)$ and $F(x,p)$.

Let's use the oscillator model to see how exactly these equations look like.

Exercise 4.1
Show that for an oscillator $v = p/m = \partial_p H$ and $F = -kx = -\partial_x H$.

Using the results of the exercise, we can conclude that for the oscillator the equations of Hamiltonian dynamics are

$$\partial_t x = \partial_p H\,, \tag{4.5}$$
$$\partial_t p = -\partial_x H\,. \tag{4.6}$$

The equations (4.5) and (4.6) are called *Hamiltonian equations of motion.*

Exercise 4.2
In special theory of relativity it is shown that the energy E and momentum p of any particle are related to its mass m as follows:

$$m^2 = E^2 - p^2\,.$$

(Special units must be used for this equation to hold. In these special units all velocities are measured as the fractions of the speed of light, while energy, momentum, and mass are all measured in the same units.)

Starting from the Hamiltonian of a relativistic particle

$$H^2 = p^2 + m^2\,,$$

show that the momentum depends on velocity as

$$p = \frac{mv}{\sqrt{1-v^2}}\,.$$

Then show that momentum and energy are related as $p = Ev$.

4.5.3 Solving Oscillator Equations

We will now find the exact time dependence of both position x_t and momentum p_t of the oscillator. To do that, we will need to take another look at the evolution of the state of the oscillator in phase space.

The state of an oscillator corresponds to a point in the phase space. This point can be mathematically represented either as a vector $|\xi\rangle$ connecting the origin and the point, or as a pair of values (x, p) . Two descriptions are equally valid. Moreover, the pair of values (x, p) can be considered as the components of the vector $|\xi\rangle$.

As the time progresses, the position and momentum of the oscillator change, but the tip of the arrow $|\xi\rangle$ remains on the ellipse, corresponding to a constant energy H. The axes of "ordinary" phase space have different physical units, whereas the "usual" Cartesian axes (x, y) have the same units and are equivalent in their meaning. It is convenient to temporarily introduce *normalized* energy, position, and momentum.

First, let us express the energy of the oscillator in terms of the rest-energy of the electron $E_e = m_e c^2$. Then the Hamiltonian of the oscillator (its total energy) can be written as $H = \bar{H} E_e$. If the rest-energy and Hamiltonian are measured in Joules, then $\bar{H}$ is a number without units. (COOKIES?)

Next, we will introduce a "scale" for position of the oscillator. Specifically, we will denote $x_e = \sqrt{2E_e/k}$ as the amplitude of the oscillation when the total energy is equal to E_e. This amplitude is measured in meters. Then the displacement can be written as $x = \bar{x} x_e$, where $\bar{x}$ is a number without units.

Finally, we will introduce a "scale" for momentum of the oscillator: $p_e = \sqrt{2mE_e}$ as the amplitude of the oscillation when the total energy is equal to E_e . (*Note*: the mass m in $\sqrt{2mE_e}$ is the mass of the body attached to the spring, *not* the mass of the electron) The "scale" p_e is measured in kilograms times meters per second – the usual units for momentum. Therefore, the momentum of the oscillator can be written as $p = \bar{p} p_e$, where $\bar{p}$ is a number without units.

Substituting $H = \bar{H} E_e$, $p = \bar{p} p_e$, and $x = \bar{x} x_e$ into the expression for the Hamiltonian, we obtain

$$\bar{H} E_e = \frac{p_e^2}{2m} \bar{p}^2 + \frac{k x_e^2}{2} \bar{x}^2 = E_e \bar{p}^2 + E_e \bar{x}^2 ,$$

from which follows a very simple relationship between pure numbers: $\bar{H} = \bar{p}^2 + \bar{x}^2$. This equation describes a circle in *normalized phase space*

$(\bar{x}, \bar{p})$. The tip of the *normalized state* vector $|\bar{\xi}\rangle = (\bar{x}, \bar{p})$ performs clock-wise circular motion. If we denote the magnitude of the angular speed of this motion as ω, then we can use the familiar equation for the circular motion:

$$\partial_t |\bar{\xi}\rangle = -\omega \, \widehat{J} \, |\bar{\xi}\rangle \, .$$

The minus sign in the right-hand side is due to the clock-wise rotation of the state vector $|\bar{\xi}\rangle$.

The left side of the last equation is a two-component vector $(\partial_t \bar{x}, \partial_t \bar{p})$. The right hand side is also a vector with components $-\omega \ \widehat{J} \ |\bar{\xi}\rangle = (\omega\bar{p}, -\omega\bar{x})$. The equality of vectors means the equality of their components:

$$\partial_t \bar{x} = \omega\bar{p} \quad \text{and} \quad \partial_t \bar{p} = -\omega\bar{x} \, .$$

Let's examine the equality $\partial_t \bar{x} = \omega\bar{p}$. The left hand side can be expanded as follows:

$$\partial_t \bar{x} = \frac{\delta\bar{x}}{\delta t} = \frac{\delta(x/x_e)}{\delta t} = \frac{1}{x_e}\frac{\delta x}{\delta t} = \frac{v}{x_e} \, .$$

The right hand side can be written as $\omega\bar{p} = \omega\frac{p}{p_e} = \frac{\omega m v}{p_e}$. We showed that

$$\frac{v}{x_e} = \frac{\omega m v}{p_e}$$

and consequently, $\omega = p_e/(m x_e)$. The conclusion is very important: *The angular speed of rotation of normalized state arrow for harmonic oscillator is constant.* The oscillator returns into its initial state with the period $T = 2\pi/\omega$.

When we plug in the expression for x_e and p_e in terms of the energy E_e and the parameters of the oscillator k and m, we will arrive at the following equations for the frequency and period of oscillatory motion:

$$\omega = \sqrt{\frac{k}{m}} \quad \text{and} \quad T = 2\pi\sqrt{\frac{m}{k}} \, .$$

Now we can write the components of the normalized state vector as

$$\bar{x} = \sqrt{\bar{H}}\cos(\omega t) \quad \text{and} \quad \bar{p} = -\sqrt{\bar{H}}\sin(\omega t) \, .$$

The minus sign for momentum comes from the fact that the "circular motion" in normalized phase space is clockwise and $\omega < 0$.

Going back to "normal" energy, position, and momentum is easy.

Indeed, we first find $x_t = x_e\sqrt{H/H_e}\cos(\omega t)$ which simplifies to simple harmonic motion:

$$x_t = \sqrt{2H/k}\cos(\omega t)\,.$$

Similarly for momentum: $p_t = -\sqrt{2mH}\sin(\omega t)$.

Exercise 4.3

Show that for harmonic oscillator

$$\Delta x = \sqrt{\langle x^2\rangle - (\langle x\rangle)^2} = \sqrt{H/k}\,,$$

and

$$\Delta p = \sqrt{\langle p^2\rangle - (\langle p\rangle)^2} = \sqrt{mH}\,.$$

Then show that $\Delta x \Delta p = H/\omega$.

4.6 Lagrangian

Lagrangian of a physical system is a special function of its coordinates and velocity that captures some aspect of energy, not covered by the total energy or Hamiltonian. For many systems Lagrangian describes the *imbalance* of kinetic energy over the potential energy. For example, the Lagrangian of the oscillator is

$$L = E_k - E_p = \frac{mv^2}{2} - \frac{kx^2}{2}\,. \tag{4.7}$$

Unlike total energy, Lagrangian is generally not conserved.

Exercise 4.4

Using the results for x_t and p_t from Hamiltonian dynamics for the oscillator, find the explicit form of its Lagrangian as the function of time.

The units for Lagrangian are the same as the units for energy or Hamiltonian (Joules in International System SI), but the meaning and the role of Lagrangian is what sets it apart from other functions of the state of a mechanical system. Lagrangian is used to find the *equations of motion* for the system. For each independent coordinate (e.g. x, y, or z) one finds a

separate equation of motion using Lagrangian. Let's see how this works for the oscillator.

The first step is to extract momentum $p = mv$ from the Lagrangian. Looking at the expression (4.7), we find $p = \partial_v L$. Next, we should find the "force" acting on the body. The force will allow us write down Newton's second law in the form $F = \partial_t p$. Again, from the expression (4.7), we find $F = -kx = \partial_x L$.

Finally, rewriting $F = \partial_t p$ in terms of the Lagrangian, we arrive at Euler-Lagrange equation:

$$\partial_t \left(\partial_v L\right) = \partial_x L \,.$$

The dynamical equations for a general system will have the same form.

> ***Lagrangian in Qoordinates***
> The power of Lagrange approach to mechanics lies in its indifference to the type of coordinates used to describe mechanical system. It is often convenient to use some *generalized coordinate* q instead of Cartesian coordinate x (or y and z). *Generalized velocity* is then $\nu = \partial_t q$. In terms of generalized variables, Euler-Lagrange equations still have the same form:
>
> $$\partial_t \pi = \partial_q L$$
>
> where $\pi = \partial_\nu L$ is *generalized momentum.*

4.6.1 Stationary Action Principle

Euler-Lagrange equations — the equations of motion for a system with specified Lagrangian $L(x, v)$ — are more rigorously derived using an important physical principle known as the *Stationary Action Principle*. Sometimes it is called *"principle of least action"* and has a special case known as *"principle of least time"*. However, the proper name is the stationary action principle. To understand the idea behind the stationary action principle we must recall the concept of a functional, and in particular the *action functional* .

Although mathematically Lagrange function $L(x, v)$ depends on two inputs – position and velocity – it is usually transformed into a function of time only L_t and then used to calculate an imporant physical quantity called *action*. We will study a specific example of this below.

Simply speaking, action is the *imbalance of energies accumulated*

during the particular motion of a system. In practice it works as follows: One chooses a particular way a mechanical system moves by choosing a particular dependence of position on time x_t. This function immediately determines the velocity $v(t) = \partial_t x$. Then we can calculate kinetic and potential energies and corresponding Lagrange function as a function of time

$$L_t = E_k(t) - E_p(t)\,.$$

With this function, we can calculate action – the total accumulated imbalance of energies – during a specific period of time:

$$A = \int \delta t L_t\,.$$

> ***Stationary Time Principle***
> When a system has constant Lagrange function, then the total action becomes proportional to total time. In this case the principle of least action is known as the *principle of extreme (least or maximal) time.*

One can try *any type of physically allowable motion* x_t and calculate the total action A. Different ways of motion will result in different values for the total action. Turns out, there is one unique function x_t^* for which the value of action A is *stationary* or *extreme* – either maximal or minimal and *insensitive to small deviations* of the motion x_t from its "true" form x_t^*. This is the essense of the *stationary action principle.* It is better to demonstrate it using an example.

Vertical Motion

Consider a body moving vertically. We can imagine two different scenarios: 1) Motion with constant acceleration (e.g. free fall) and 2) Motion with constant speed.

If the initial height is h, velocity zero, and the acceleration a, then the position along the vertical axis y and corresponding velocity are known:

$$y_a = h - at^2/2\,, \qquad v_a = -at\,.$$

The body will reach the "ground" ($y = 0$) at time $T = \sqrt{2h/a}$.

Imagine the second body that begins and ends its motion simultaneously with the first body but moving with constant speed $u = h/T$. Then

we can write

$$y_c = h - ut\,, \qquad v_c = -u\,.$$

Let's denote the first type of motion as $q_1(t)$ and the second as $q_0(t)$. We can consider other types of motion, as long as they start at $y = h$ when $t = 0$ and end at $y = 0$ when $t = h$. For example, we can consider the following motion:

$$q_\alpha(t) = \alpha q_1 + (1-\alpha)q_0\,, \qquad \alpha \in [0,1]\,.$$

It is an type of motion somewhere in between the two variants mentioned above. For the value $\alpha = 0$ of the parameter we recover the motion with constant speed $q_0(t)$, while for $\alpha = 1$ we get the uniformly accelerated motion $q_1(t)$ with zero initial velocity.

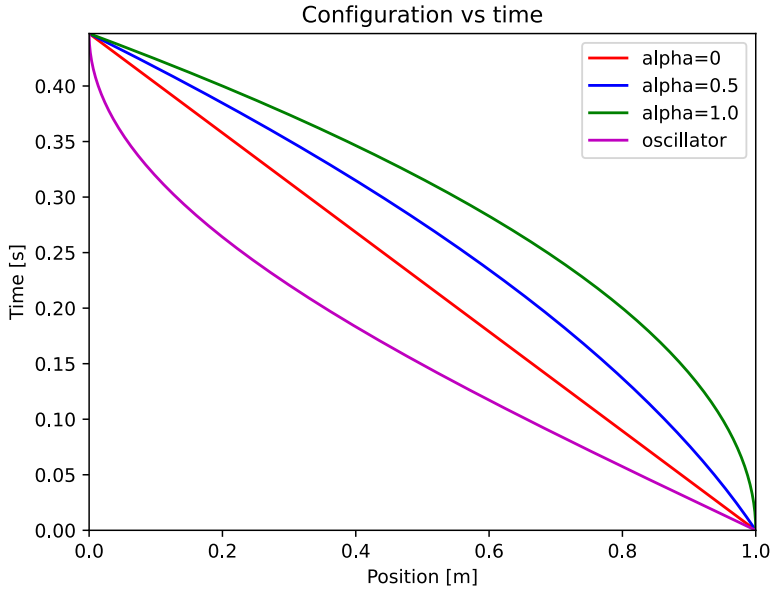


Fig. 4.7: Different types of vertical motion in Lagrange picture. Particles start and stop at the same times and in the same places, moving between initial and final configurations according to different equation $q(t)$.

It is not difficult to see that the velocity for this general motion is

given by similar combination of velocities:

$$v_\alpha(t) = \alpha v_a + (1-\alpha)v_c\,.$$

Let's calculate the Lagrange function for a body moving freely, without any forces acting on it. Then the Lagrange function is simply its kinetic energy:

$$L(t) = \frac{mv_\alpha^2}{2} = \frac{m}{2}\left[\alpha^2 v_a^2 + (1-\alpha)^2 v_c^2 + 2\alpha(1-\alpha)v_a v_c\right].$$

Plugging in the expressions for velocity, we arrive at

$$L(t) = \frac{m}{2}\left[\alpha^2 a^2 t^2 + (1-\alpha)^2 u^2 + 2\alpha(1-\alpha)aut\right].$$

Now we can calculate the total action accumulated during the motion from $t = 0$ to $t = T$:

$$A = \int L(t)\delta t = \alpha^2 S_1 + (1-\alpha)^2 S_2 + \alpha(1-\alpha)S_3\,.$$

Here we denoted

$$S_1 = \frac{ma^2}{2}\int t^2\delta t\,, \qquad S_2 = mu^2\int \delta t\,, \qquad S_3 = 2mau\int t\delta t\,.$$

Examining the expression for the total action, we see that A depends on the "mixing" parameter α in a quadratic way:

$$A(\alpha) = (S_1 + S_2 - S_3)\alpha^2 + (S_3 - 2S_2)\alpha + S_2\,.$$

The sums can be evaluated:

$$S_1 = \frac{ma^2}{2}\frac{T^3}{3}\,, \qquad S_2 = mu^2 T = \frac{mh^2}{T}\,, \qquad S_3 = mauT^2 = mahT\,.$$

Recalling that $T = \sqrt{2h/a}$ and therefore $h = aT^2/2$, we find

$$S_3 - 2S_2 = (ma^2T^3/2) - 2ma^2T^4/(4T) = 0\,.$$

The coefficient in front of α^2 is

$$S_1 + S_2 - S_3 = \frac{ma^2T^3}{6} + \frac{ma^2T^3}{4} - \frac{ma^2T^3}{2} = -\frac{ma^2T^3}{12}\,.$$

Finally, the total action depends in the parameter α as

$$A = \frac{ma^2T^3}{12}(3 - \alpha^2)\,.$$

To find the condition for extremal/stationary action, we need to find α that maximizes or minimizes the action. Since $A(\alpha)$ is the inverted parabola with maximum at $\alpha = 0$, the maximal action is achieved for the motion $q_0(t)$ with constant speed without acceleration and forces.

Exercise 4.5

Consider the Lagrange function for a body moving under the force of gravity:

$$L = \frac{mv^2}{2} - mgq\,.$$

Calculate $L(t)$ for $q_\alpha(t)$ and then calculate total action accumulated between $t = 0$ and $t = T$. Find α for which the action $A(\alpha)$ becomes stationary.

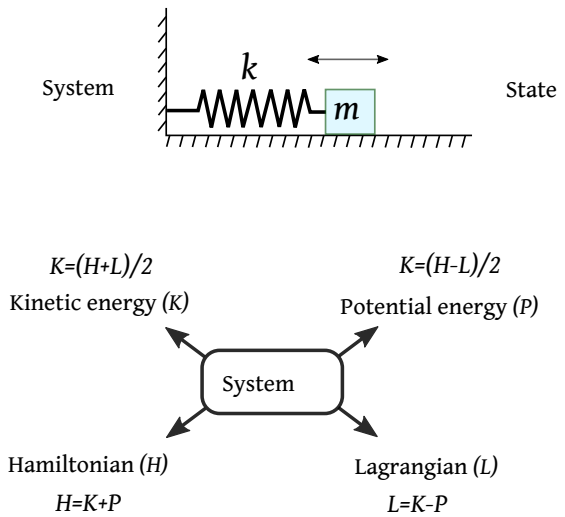


Fig. 4.8: System can be described either by kinetic and potential energies, or Hamiltonian, or Lagrangian.

Exercise 4.6

Consider the following ways of traveling from the height $y = h$ to the ground $y = 0$ in time T:

$$q_1(t) = h - gt^2/2\,,$$

$$q_2(t) = h(1 - t/T)\,,$$

$$q_3(t) = h\left(1 - \sin\frac{\pi t}{2T}\right)\,,$$

$$q_4(t) = h\frac{ee^{-t/T} - 1}{e - 1}\,,$$

and

$$q_5(t) = h(1 - t/T)^2\,.$$

4.6.2 Summary of Three Mechanics

Let's review what we've learned about three different approaches to study dynamics.

State is $|\xi\rangle = (q, u)$ where q is the generalized coordinate and $u = \partial_t q$ is *generalized velocity*. Generalized momentum:

$$\pi = \partial_u L\,,$$

Euler-Lagrange equation:

$$\partial_t \pi = \partial_q L\,.$$

4.7 Field

The *field* concept is extremely important for modern physics, both classical and quantum.

In physics, *field* is a *dynamical system* with infinite number of degrees of freedom. It's dynamics can be studied using either Lagrangian or Hamiltonian approach.

4.8 Ideal Versus Real

An action of an operator F on arrows can be represented symbolically as an equation.

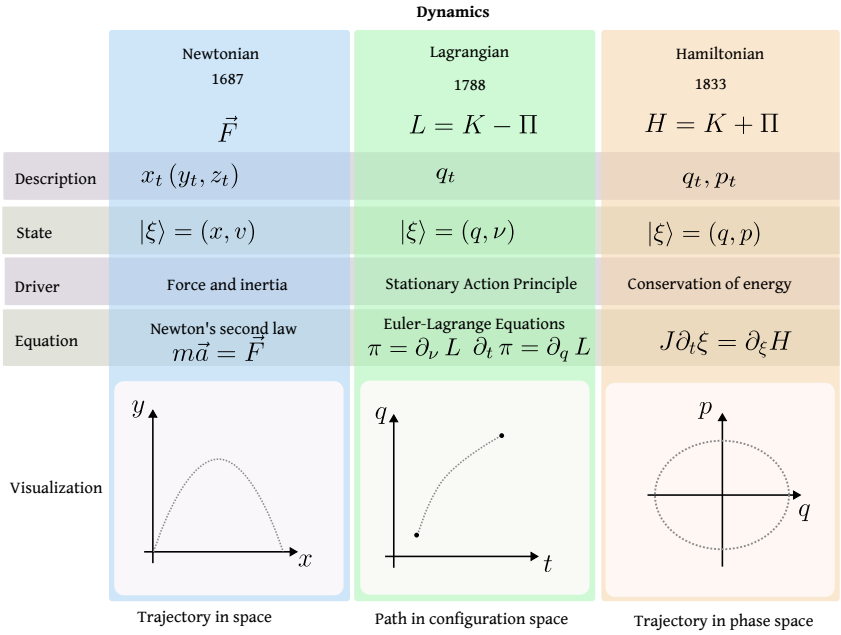
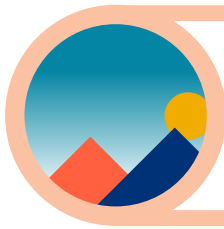


Fig. 4.9: Summary of three different approaches to problems of motion.

Chapter Highlights

- *Operators extends the idea of functions.*
- *Numeric functions (e.g.,* $\sin x$*) act on numbers and yield other numbers. Operators may act on vectors to yield other vectors or numbers.*
- *Linear operators represent the simplest and yet powerful class of operators on vectors.*
- *Linear operators can be represented graphically or symbolically.*



5. Quantum Physics

The first type of operators – and corresponding tensors – that we encountered has a simple type:

$$\hat{L}\ \vec{a} = \vec{b}\,.$$

It is a linear unary function mapping vectors into vectors.

> ☑ ***Prerequisite Knowledge***
> To fully understand the material of this chapter, readers should be comfortable with the following concepts:
> - State
> - Dynamical equations

5.1 Quantum System

We are looking for a binary operator $\hat{\sigma}$ that yields a number based on two vectors:

$$|\sigma\rangle\langle\sigma|\,\vec{a}\,\vec{b} = x\,.$$

5.2 Fundamental Randomness

5.3 Quantum State

We are looking for a binary operator $\hat{\sigma}$ that yields a number based on two vectors:

$$|\sigma\rangle\langle\sigma|\,\vec{a}\,\vec{b} = x\,.$$

5.3.1 Superposition

Suppose we measure the energy of a quantum system (e.g. a hydrogen atom) and find that it takes on discrete values E_1, E_2, E_3, and so on. A distinct quantum state $|e_1\rangle$, $|e_2\rangle$, $|e_3\rangle$, and so on, is associated with each energy value.

If a long series of measurements always yields the same energy value E_k, we conclude that the system was prepared in the state of *definite* energy $|e_k\rangle$. If the results of a long series of measurements are random, then the initial state of atoms can not be the state of a definite energy. In practice, a long series of measurements of *identically prepared* atoms reveals certain *statistical* pattern. Specifically, for a number of measurement N, the energy E_1 results in N_1 random outcomes, the energy E_2 results in N_2 random outcomes and so on. One can speak of the *probability* of obtaining the result E_1, defined as the *relative frequency* $p_1 = N_1/N$ of occurences of E_1; similary for other results. Generally, the probability of obtaining the result E_k is $p_k = N_k/N$.

If the probabilities $(p_1, p_2, p_3, \ldots, p_k)$ are *reproducible* (the same set of probabilities in different repeated long series of measurements), then the state of system can be characterized by the combination of energy values and their probabilities:

$$|\xi\rangle \longrightarrow \{(E_1, p_1), (E_2, p_2), (E_3, p_3), \ldots, (E_k, p_k)\}\,.$$

If there is a one-to-one correspondence $E_k \leftrightarrow |e_k\rangle$ between the energy and the state, then the state $|\xi\rangle$ can be said to be *determined* by (or is a function of) the set of pairs $(p_i, |e_i\rangle)$:

$$|\xi\rangle \longleftrightarrow \{(p_1, |e_1\rangle), (p_2, |e_2\rangle), (p_3, |e_3\rangle), \ldots, (p_k, |e_k\rangle)\}\,.$$

The *simplest* function that constructs one vector from other vectors is a *linear combination*. We can try using such a function to express the state $|\xi\rangle$ in terms of the states with definite energy $|e_i\rangle$ as follows:

$$|\xi\rangle = p_1|e_1\rangle + p_2|e_2\rangle + p_3|e_3\rangle + \ldots p_k|e_k\rangle\,.$$

There is no guarantee that this approach will be effective. In fact, the expression given above is *not the one* used in quantum theory, but it is not far from the "proper" quantum form.

Mixed State
The expression for the state as a linear combination of other states with coefficients equal to corresponding probabilities *can* be applied in systems in so-called *mixed state*.

$$\widehat{\rho} = p_1\ \widehat{\rho}_1 + p_2\ \widehat{\rho}_2 + \ldots + p_k\ \widehat{\rho}_k\ .$$

Every state can be viewed as a linear combination – called *superposition* – of some other states:

$$|\psi\rangle = c_1|\phi_1\rangle + c_2|\phi_2\rangle + \ldots + c_k|\phi_k\rangle\,.$$

This is analogous to the representation of arrow-vectors in terms of some basis.

Born Rule

5.3.2 States Overlap

$$\langle\psi|\phi\rangle.$$

5.3.3 Pure and Mixed States

State Purification

It is possible to "upgrade" a mixed state of a quantum sustem S given by a density operator $\widehat{\rho}$ to a pure state $|\Psi\rangle$. The mathematical procedure is called *purification*. Physically, the operation means finding a larger system S_L which contains S as its "part" and can be described using a pure state vector $|\Psi\rangle$.

Purification can always be achieved. One natural choice of a "larger" quantum system S_L can be a system consisting of a pair of S-like systems. As an example, a mixed state of a qubit can be purified to a state of qubit pair.

5.3.4 Fidelity

When the state of a quantum system cannot be described using a state vector $|\psi\rangle$, we need to use a more general approach – *state operator* or *density operator* $\widehat{\rho}$.

How do we compare two states $\widehat{\rho}$ and $\widehat{\sigma}$ for similarity? A useful measure of similarity in this case is called *fidelity* and has the following

definition:

$$\mathcal{F}(\widehat{\rho}, \widehat{\sigma}) = \mathtt{Tr}\sqrt{\sqrt{\widehat{\rho}}\ \widehat{\sigma}\ \sqrt{\widehat{\rho}}}\,.$$

This complicated definition captures almost the same idea as the scalar product. In fact, for pure states $\widehat{\rho} = |\psi\rangle\langle\psi|$ and $\widehat{\sigma} = |\phi\rangle\langle\phi|$ it returns the absolute value of the scalar product $|\langle\psi|\phi\rangle|$.

Using fidelity allows comparing pure states and mixed states. Indeed, for a pure state $\widehat{\rho} = |\psi\rangle\langle\psi|$ (a projector) the square root is $\widehat{\rho}$, and

$$\widehat{\rho}\widehat{\sigma}\widehat{\rho} = \langle\psi|\ \widehat{\sigma}\ |\psi\rangle\ \widehat{\rho}\ .$$

Taking the square root of the last expression gives

$$\alpha\,\widehat{\rho}\,,$$

where $\alpha = \sqrt{\langle\psi|\ \widehat{\sigma}\ |\psi\rangle}$ is a number. Finally, using the fact that $\mathtt{Tr}\ \widehat{\rho} = 1$, we obtain

$$\mathcal{F}(\widehat{\rho}, \widehat{\sigma}) = \sqrt{\langle\psi|\ \widehat{\sigma}\ |\psi\rangle}\,.$$

Recall that $\langle\psi|\ \widehat{\sigma}\ |\psi\rangle$ is the expectation value of the operator $\widehat{\sigma}$ in the state $|\psi\rangle$.

Exercise 5.1
Prove that the definition of fidelity implies that it is symmetric in its arguments.

5.4 Quantum Dynamics

We are looking for a binary operator $\widehat{\sigma}$ that yields a number based on two vectors:

$$|\sigma\rangle\langle\sigma|\,\vec{a}\,\vec{b} = x\,.$$

5.5 Quantum Hamiltonian

We are looking for a binary operator $\widehat{\sigma}$ that yields a number based on two vectors:

$$|\sigma\rangle\langle\sigma|\,\vec{a}\,\vec{b} = x\,.$$

5.6 Quantum Bit

Any quantum system with two active states is called a *qubit*. The state with lower energy is usually called *ground state* and denoted as $|g\rangle$ or $|0\rangle$ (zero). The state with higher energy is usually called *excited state* and denoted as $|e\rangle$ or $|1\rangle$ (one). The notation $|0\rangle, |1\rangle$ is used in the field of quantum information and computation.

If the energy of the ground and excited states are E_g and E_e, respectively, then the Hamiltonian of a qubit can be written using projectors

$$\widehat{H} = E_g|g\rangle\langle g| + E_e|e\rangle\langle e|\,.$$

It requires an energy $\Delta E = E_e - E_g$ to excite the qubit from the lower energy state to the higher energy state. This energy may come from a quantum of electromagnetic field oscillating with frequency $\omega = \Delta E/\hbar$.

5.6.1 Flipping Operator

Transition between the states of a qubit can be described mathematically using operators that map one state into another. For example, an operator $\widehat{F}$ that *flips* states must do the following:

$$\widehat{F}\ |0\rangle = |1\rangle\,, \quad \widehat{F}\ |1\rangle = |0\rangle\,.$$

Such operator can be easily built from the tensor products:

$$\widehat{F} = |1\rangle\langle 0| + |0\rangle\langle 1|\,.$$

Each term in this sum is useful in quantum theory. The first term is called *raising operator* and is denoted as $\widehat{\sigma}_+ = |1\rangle\langle 0|$. The second term is called *lowering operator* and is denoted as $\widehat{\sigma}_- = |0\rangle\langle 1|$. Apparently, the raising operator excites the qubit from the ground state, while the lowering operator brings the qubit down from the excited state.

Exercise 5.2
Calculate $\widehat{F}^2$.

Exercise 5.3
Calculate (a) $\widehat{\sigma}_+\widehat{\sigma}_+$; (b) $\widehat{\sigma}_-\widehat{\sigma}_-$; (c) $\widehat{\sigma}_+\widehat{\sigma}_-$; (d) $\widehat{\sigma}_-\widehat{\sigma}_+$.

Exercise 5.4
Show that $\widehat{\sigma}_+\widehat{\sigma}_- + \widehat{\sigma}_-\widehat{\sigma}_+ = \widehat{I}$, where $\widehat{I}$ is the identity operator.

Exercise 5.5
Show that the qubit Hamiltonian can be written in terms of the raising and lowering operators as follows:

$$\widehat{H} = \hbar\omega\left(\widehat{\sigma}_+\widehat{\sigma}_- + \epsilon\,\widehat{I}\right),$$

where $\epsilon = E_g/\Delta E$.

5.6.2 Number Operator

The operator $\widehat{n} = \widehat{\sigma}_+\widehat{\sigma}_-$ is called *number operator* for the following reason. First, note that $\widehat{\sigma}_+\widehat{\sigma}_- = |1\rangle\langle 1|$ is the projector on the excited state of qubit.

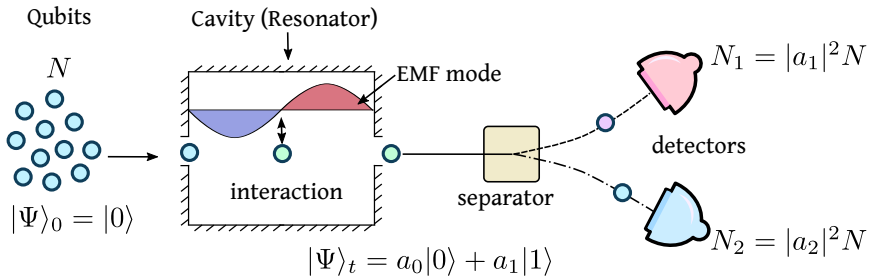


Fig. 5.1: Qubits initially in the ground state $|0\rangle$ travel through a cavity resonator with an electromagnetic field mode attuned to the qubits transition energy $\Delta E = \hbar\omega$. After interaction, the state of each qubit changes to $|\Psi_t\rangle$. Then the qubits are "measured"/separated into two groups, based on their final state.

Next, consider an experiment schematically shown in Figure 5.1. In this experiment a large number N of qubits start in the ground state $|0\rangle$ and go through a region (cavity) where they can interact with an oscillating electromagnetic field (mode). After leaving the cavity, each qubit goes through a special device which splits the beam into two parts, depending on the measured state of a qubit. The top detector detects N_1 qubits in state $|1\rangle$, the bottom detector detects N_2 qubits in ground state. The N_1 qubits correspond to the number of energy quanta absorbed from

cavity. This number can be expressed as

$$N_1 = N|a_1|^2 = N\langle\Psi_t|\,\widehat{n}\,|\Psi_t\rangle\,.$$

In other words, the expectation value of the operator $\widehat{n}$ determines the number of energy quanta absorbed from the mode of electromagnetic field inside the cavity.

5.7 Quantum Oscillator

The *principle of the quantization of action* can be applied to harmonic oscillator. The result is the quantization of energy levels.

The energy of a harmonic oscillator can be expressed in terms of the maximum momentum p_m or in terms of the maximum displacement x_m:

$$H = \frac{p_m^2}{2m} \quad \text{or} \quad H = \frac{kx_m^2}{2}\,.$$

Multiplying these two equalities and recalling that $\omega^2 = k/m$, we obtain

$$H = \frac{\omega x_m p_m}{2}\,.$$

The path which the state vector $|\xi\rangle = (x, p)$ follows in phase space is an ellipsis with the major semi-axes x_m and p_m. The area of this ellipsis is $A = \pi x_m p_m$. Therefore, the connection between the energy of harmonic oscillator and the area is given by

$$H = \frac{\omega}{2\pi}A\,.$$

The area A is a physical quantity with the units of action.

As shown in Figure 5.2(a), areas in phase space have the smallest size limited by the elementary quantum of action h – known as Planck constant. The quantization of action and, consequently, the quantization of phase-space area, has two important implications for harmic oscillator.

First, every time an oscillator absorbs some energy ΔE, the maximum deviation and the maximum momentum increase. The ellipsis in phase space increases its area. But since the area in phase space can't grow continiously–changes in discrete quanta $\delta A = h$–we must have discreete changes in energy. Second, the existence of the elementary quantum

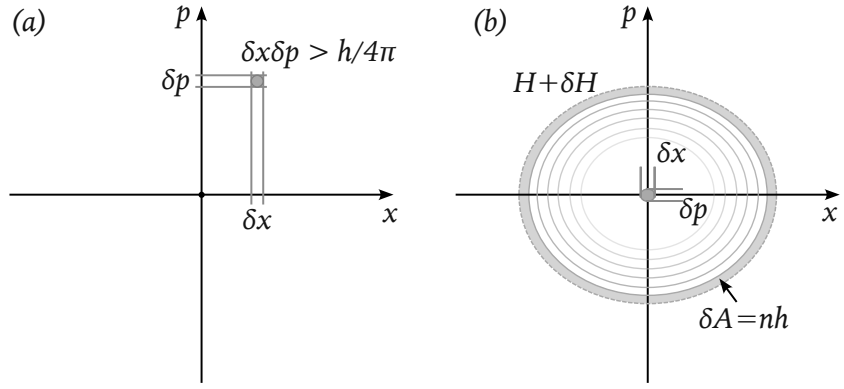


Fig. 5.2: Areas of phase-space regions have the units of action. Quantization of action implies quantization of phase-space area. (a) The smallest area in phase space is limited by the fundamental quantum of action h – Planck's constant. (b) Area of the ellipsis inside the path of harmonic oscillator is proportional to its energy. Quantization of area leads to the quantization of energy of harmonic oscillator.

of action and the smallest are in phase space, require that the lowest energy state of harmonic oscillator is described not by a point in phase space, but by an elementary ellipsis such that $A_0 = \delta x \delta p \propto h$. Putting these two ideas together, we conclude that the area of the ellipsis can be written as

$$A_n = A_0 + nh\,.$$

The energy of the oscillator then takes the form

$$H = n\hbar\omega + E_0\,,$$

where $\hbar = h/2\pi$ is called *reduced Planck's constant*, and E_0 is the lowest energy of the harmonic oscillator. From the expression for H follows that harmonic oscillator can be in a countable set of states, growing in energy from E_0 by a fixed step $\hbar\omega$.

The energy of the lowest state can be written in terms of the step size $\hbar\omega$: $E_0 = e_0\hbar\omega$, where e_0 is some number (it will be found later). Finally, we can write the energy of harmonic oscillator as follows:

$$H = \hbar\omega(n + e_0)\,.$$

5.7.1 Hamiltonian Operator

For any quantum system with descrete energy states $E_0, E_1, E_2, \ldots, E_n \ldots$ the Hamiltonian operator can be written in terms of projectors:

$$\widehat{H} = \int E_k |k\rangle\langle k| \,, \quad k = 0, 1, 2, \ldots, n \ldots$$

For harmonic oscillator $E_k = E_0 + k\hbar\omega$ for $n > 1$ and the Hamiltonian operator can be written as follows

$$\widehat{H} = \int (E_0 + k\hbar\omega) |k\rangle\langle k| \,.$$

The number k tells how many excitations quantum oscillator absorbed to reach the energy state $|k\rangle$. Opening the parentheses and recalling that

$$\int |k\rangle\langle k| = \widehat{I} \,,$$

we obtain

$$\widehat{H} = E_0 \, \widehat{I} + \hbar\omega \int k |k\rangle\langle k| \,.$$

This expression is very similar to the Hamiltonian of a qubit

$$\widehat{H}_{qb} = E_g \, \widehat{I} + \hbar\omega \, \widehat{n}$$

where $\widehat{n} = \widehat{\sigma_+}\widehat{\sigma_-}$ is a number operator. The similarity is not accidental, as the operator $\widehat{n} = \int k |k\rangle\langle k|$ plays the role of the number operator. Indeed, it is easy to check by direction application that:

$$\widehat{n} \;\; |n\rangle = n|n\rangle \,.$$

In other words, the energy states $|n\rangle$ of harmonic oscillator, are the eigen-states of the number operator $\widehat{n}$ with the eigen-value n corresponding to the number of excitation level.

Exercise 5.6
Prove that $\widehat{n} \;\; |n\rangle = n|n\rangle$ by direction application of the operator $\widehat{n} = \int k |k\rangle\langle k|$.

The expression for the number operator $\widehat{n}$ can be obtained in a different way. First note that

$$\widehat{H} \;\; |n\rangle = E_n |n\rangle \,, \qquad \text{where } E_n = E_0 + n\hbar\omega \,.$$

From this follows

$$(\widehat{H} - E_0\,\widehat{I})\,|n\rangle = n\hbar\omega\,|n\rangle\,,$$

and, consequently,

$$\frac{(\widehat{H} - E_0\,\widehat{I})}{\hbar\omega}\,|n\rangle = n\,|n\rangle\,.$$

The operator on the left hand side of this equation is the number operator $\widehat{n}$. It can be simplified once we recall that

$$\widehat{H} = \int E_k |k\rangle\langle k| \quad \text{and} \quad \widehat{I} = \int |k\rangle\langle k|\,.$$

Using these relations, we first write

$$\widehat{H} - E_0\,\widehat{I} = \int (E_k - E_0)|k\rangle\langle k|\,.$$

Then, remembering that $E_k = E_0 + k\hbar\omega$, we immediately arrive at

$$\widehat{n} = \frac{(\widehat{H} - E_0\,\widehat{I})}{\hbar\omega} = \int k|k\rangle\langle k|\,.$$

Thus, the operator of quantum harmonic oscillator can be written in the following form:

$$\widehat{H}_{osc} = E_0\,\widehat{I} + \hbar\omega\,\widehat{n}\ .$$

5.7.2 Ladder Operators

The number operator for qubit could be expressed as the product of two simple operators that raised or lowered qubit states:

$$\widehat{n} = \widehat{\sigma}_+\widehat{\sigma}_-\ .$$

The idea of raising and lowering states is also applicable to harmonic oscillator. Similar to qubit, we can write such operators as tensor products:

$$\widehat{a}_+ = |n+1\rangle\langle n| \quad \text{and} \quad \widehat{a}_- = |n-1\rangle\langle n|\,.$$

Unfortunately, these operators will act properly only on the state $|n\rangle$.

Exercise 5.7

Evaluate (a) $\widehat{a}_+\ |n\rangle$; (b) $\widehat{a}_-\ |n\rangle$; (c) $\widehat{a}_+\ |n+m\rangle$; (d) $\widehat{a}_+\ |n+m\rangle$.

It is easy to fix this problem by summing over all states:

$$\widehat{a}_+ = \int |k+1\rangle\langle k| \quad \text{and} \quad \widehat{a}_- = |0\rangle\langle 0| + \int |m-1\rangle\langle m|\,, \quad m > 0\,.$$

The first term in the expression for $\widehat{a}_-$ ensures that the vacuum state remains unchanged: $\widehat{a}_- \ |0\rangle = |0\rangle$.

Exercise 5.8
Evaluate (a) $\widehat{a}_+ \ |n\rangle$; (b) $\widehat{a}_- \ |n\rangle$.

Let's check whether $\widehat{a}_+\widehat{a}_-$ yields the number operator $\widehat{n} = \int k|k\rangle\langle k|$. Even without explicitely evaluating the composition $\widehat{a}_+\widehat{a}_-$ we can see that it is unlikely to contain the required factor k.

Exercise 5.9
Show that $\widehat{a}_+\widehat{a}_- = |1\rangle\langle 0| - |0\rangle\langle 0| + \widehat{I}$.

To find better operators for raising and lowering states of harmonic oscillator, we can taken a closer look at the qubit case. There we had $\widehat{\sigma}_+ \ |0\rangle = 1|1\rangle$ and $\widehat{\sigma}_- \ |1\rangle = 1|0\rangle$. We explicitely added "1" in front of the final states, to highlight the following property of the $\widehat{\sigma}$-operators:

$$\widehat{\sigma}_+ \ |k\rangle = \sqrt{k+1}|k+1\rangle \quad \text{and} \quad \widehat{\sigma}_- \ |k\rangle = \sqrt{k}|k-1\rangle\,.$$

Thus, we can "upgrade" the raising and lowering operators $\widehat{a}_+$ and $\widehat{a}_-$ to include the information about the state they act on. We want them to behave as follows:

$$\widehat{a}_+ \ |k\rangle = \sqrt{k+1}|k\rangle \quad \text{and} \quad \widehat{a}_- \ |m\rangle = \sqrt{m}|m-1\rangle\,.$$

Exercise 5.10
Evaluate $(\widehat{a}_+)^p \ |0\rangle$.

Exercise 5.11
(a) Show that the upgraded operators have the property

$$\widehat{a}_+\widehat{a}_- \ |m\rangle = m|m\rangle \quad m > 0\,.$$

(b) Evalulate $\widehat{a}_{-}\widehat{a}_{+}\ |m\rangle$.

Exercise 5.12
(a) Show that

$$\widehat{a}_{-}\widehat{a}_{+} - \widehat{a}_{+}\widehat{a}_{-}=\widehat{I}\ .$$

Such raising and lowering operators (also called *ladder operators*) are very useful when working with quantum harmonic oscillators. In terms of the ladder operators, the Hamiltonian of quantum oscillator is written as

$$\widehat{H}_{osc}= \hbar\omega\ \widehat{n} +E_0\ \widehat{I}\,,$$

where the number operator $\widehat{n}=\widehat{a}_{+}\widehat{a}_{-}$.

5.7.3 Conjugation

The raising operator $\widehat{a}_{+}$ can be written in terms of the tensor products:

$$\widehat{a}_{+}= \int_0 \sqrt{k+1}|k+1\rangle\langle k|\,.$$

If we limit the lowering operator to states $|m\rangle$ with $m > 0$, then it also allows a simple representation

$$\widehat{a}_{-}= \int_1 \sqrt{m}|m-1\rangle\langle m|\,.$$

By changing the summation variable $m-1 = k$ (and, therefore, $m = k+1$), we can re-write the summation over $k = 0, 1, 2\ldots$:

$$\widehat{a}_{-}= \int_0 \sqrt{k+1}|k\rangle\langle k+1|\,.$$

Now the expression for $\widehat{a}_{-}$ became similar to the expression for $\widehat{a}_{+}$, with the exception that the order of states in the tensor product is flipped:

$$|k+1\rangle\langle k| \leftrightarrow |k\rangle\langle k+1|\,.$$

This change of order of factors in a tensor product is called *conjugation*. The operators $\widehat{a}_{-}$ and $\widehat{a}_{+}$ are therefore related to each other via the *conjugation operation*. These operators are said to be *conjugates* of each other.

The relation of conjugation gives some insight into what the lowering operator $\widehat{a}_-$ does to the vacuum state:

$$\widehat{a}_- \ |0\rangle = \int_0 \sqrt{k+1}|k\rangle\langle k+1|0\rangle = 0 \int_0 \sqrt{k+1}|k\rangle = 0|\infty\rangle \,,$$

where we introduced a vector

$$|\infty\rangle = |0\rangle + \sqrt{2}|1\rangle + \sqrt{3}|2\rangle + \ldots + \sqrt{n+1}|n\rangle + \ldots$$

Obviously, $|\infty\rangle \neq |0\rangle$. The overall factor of zero negates any possible contributions of $|\infty\rangle$, making the product $0|\infty\rangle$ a special "zero vector" $|z_0\rangle$, with the natural property

$$|k\rangle + |z_0\rangle = |k\rangle \,.$$

The vector $|z_0\rangle$ does not correspond to any physical state, but represents a mathematical "zero vector". Since for all mathematical manipulations the vectors $0|\infty\rangle$ and $0|0\rangle$ are equivalent, we can express the action of the lowering operator $\widehat{a}_-$ on the vacuum state as follows:

$$\widehat{a}_- \ |0\rangle = 0|0\rangle \,.$$

Finally, the action of the number operator $\widehat{n}{=}\widehat{a}_+\widehat{a}_-$ on the vacuum state can be evaluated:

$$\widehat{a}_+\widehat{a}_- \ |0\rangle = \widehat{a}_+ \ (\widehat{a}_- \ |0\rangle) = 0(\widehat{a}_+ \ |0\rangle) = 0|1\rangle = 0|0\rangle \,,$$

here we used the mathematical equivalence of states $0|1\rangle$ and $0|0\rangle$.

Dagger Notation

The relation of conjugation between operators is denoted using a special notation. For example, if we denote the lowering operator $\widehat{a}_-$ simply as $\widehat{a}$, then its conjugate operator– raising operator– is denoted using a special "dagger" symbol as the superscript:

$$\widehat{a}_+{=}\widehat{a}^\dagger \ .$$

The use of dagger notation is standard in quantum theory.

Let's use the dagger notation to summarize the basis facts about the ladder operators, the number operator, and the Hamiltonian of

quantum oscillator. First, raising and lowering properties:

$$\hat{a}\ |n\rangle = \sqrt{n}|n-1\rangle\,, \qquad \hat{a}^\dagger\ |n\rangle = \sqrt{n+1}|n+1\rangle\,.$$

Second, number operator and commutator:

$$\hat{a}^\dagger\,\hat{a}\ |n\rangle = n|n\rangle\,, \qquad \hat{a}\,\hat{a}^\dagger - \hat{a}^\dagger\,\hat{a}{=}\hat{I}\ .$$

Finally, conjugation relation between the ladder operators:

$$\hat{a}\xrightarrow{\dagger}\hat{a}^\dagger\ .$$

Normal Order

Exercise 5.13

Ladder operators are used many important applications of quantum theory. Often one encounters expressions with several operators in no particular order, for example $\hat{X}{=}\hat{a}^\dagger\,\hat{a}^2\,\hat{a}^\dagger\,\hat{a}$. For calculations it is necessary to rearrange these operators into a *normal order* where all raising operators appear on the left, before the lowering operators.

Use the commutation relation $\hat{a}\,\hat{a}^\dagger - \hat{a}^\dagger\,\hat{a}{=}\hat{I}$ to put $\hat{X}$ into a normal order.

5.7.4 Canonical Commutation

The Hamiltonian operator for quantum harmonic oscillator can be written in different ways. One way relies on energy eigen-values E_k:

$$\hat{H}{=}\int_0 E_k|k\rangle\langle k|\,.$$

Another way utilizes raising and lowering operators:

$$\hat{H}{=}\,\hbar\omega\,\hat{a}^\dagger\,\hat{a}\,{+}E_0\,\hat{I}\ .$$

However, the starting point was the expression in terms of position and momentum. The question then becomes whether we can introduce *position and momentum operators* such that for harmonic oscillator we get

$$\hat{H}{=}\,\frac{\hat{p}^2}{2m}+\frac{m\omega^2\,\hat{x}^2}{2}\,.$$

We already saw in Exercise X the hint that some relationship must exist between the operators $\widehat{a}$, $\widehat{a}^\dagger$ and $\widehat{x}$, $\widehat{p}$. Such relationship must be linear in order to transform the expression for $\widehat{H}$ quadratic in terms of raising and lowering operator

$$\widehat{H} = E_0\,\widehat{a}\,\widehat{a}^\dagger + (\hbar\omega - E_0)\,\widehat{a}^\dagger\,\widehat{a} = \square\,\widehat{a}\,\widehat{a}^\dagger + \square\,\widehat{a}^\dagger\,\widehat{a}$$

into the expression quadratic in terms of position and momentum

$$\widehat{H} = \square\,\widehat{p}^2 + \square\,\widehat{x}^2 \ .$$

We are thus looking for a linear transformation

$$\widehat{x} = A\,\widehat{a} + B\,\widehat{a}^\dagger \qquad \text{and} \qquad \widehat{p} = C\,\widehat{a} + D\,\widehat{a}^\dagger$$

which will lead to the Hamiltonian operator $\widehat{H} = E_0\,\widehat{a}\,\widehat{a}^\dagger + (\hbar\omega - E_0)\,\widehat{a}^\dagger\,\widehat{a}$.

Exercise 5.14

Show that the Hamiltonian operator for harmonic oscillator in terms of the unknown coefficients A, B, C and D has the form:

$$\widehat{H} = \left(\frac{C^2}{2m} + \frac{m\omega^2 A^2}{2}\right)\widehat{a}^2 + \left(\frac{D^2}{2m} + \frac{m\omega^2 B^2}{2}\right)\widehat{a}^\dagger + \\ + \left(\frac{CD}{2m} + \frac{m\omega^2 AB}{2}\right)\widehat{a}\,\widehat{a}^\dagger + \left(\frac{CD}{2m} + \frac{m\omega^2 AB}{2}\right)\widehat{a}^\dagger\,\widehat{a} \ .$$

Exercise 5.15

Using the result of the previous exercise, show that it implies that $E_0 = \hbar\omega/2$.

Exercise 5.16

Using the results of the two previous exercises, show that the four unknown coefficients A, B, C and D satisfy the following equations:

$$C^2 = -(m\omega A)^2 \ ,$$

$$D^2 = -(m\omega B)^2 ,$$

and

$$CD + (m\omega)^2 AB = m\hbar\omega .$$

Exercise 5.17

Using the result of the previous exercise, show that $CD = (m\omega)^2 AB$ (convince yourself that CD can't be $CD = -(m\omega)^2 AB$!). Then show that one possible solution is the set of coefficients:

$$A = B = \sqrt{\frac{\hbar}{2m\omega}} ,$$

and

$$C = -D = -\,\widehat{J}\sqrt{\frac{\hbar m\omega}{2}} .$$

With the steps outlined above, we obtain the following expressions for the operators of position and momentum:

$$\widehat{x} = \sqrt{\frac{\hbar}{2m\omega}}\left(\widehat{a}^\dagger + \widehat{a}\right) = x_\omega\left(\widehat{a}^\dagger + \widehat{a}\right)$$

and

$$\widehat{p} = \widehat{J}\sqrt{\frac{\hbar m\omega}{2}}\left(\widehat{a}^\dagger - \widehat{a}\right) = \widehat{J}\, p_\omega\left(\widehat{a}^\dagger - \widehat{a}\right) .$$

Using these relations, it is now easy to find so called *canonical commutation relation* for the basic physical operators of position and momentum. First, we find

$$\widehat{x}\widehat{p} = \widehat{J}\,\frac{\hbar}{2}\left(\widehat{a}^\dagger\widehat{a}^\dagger - \widehat{a}\widehat{a} + \widehat{a}\widehat{a}^\dagger - \widehat{a}^\dagger\widehat{a}\right),$$

then

$$\widehat{p}\widehat{x} = \widehat{J}\,\frac{\hbar}{2}\left(\widehat{a}^\dagger\widehat{a}^\dagger - \widehat{a}\widehat{a} + \widehat{a}^\dagger\widehat{a} - \widehat{a}\widehat{a}^\dagger\right).$$

Subtracting the latter equation from the former, we arrive at

$$\widehat{x}\widehat{p} - \widehat{p}\widehat{x} = [\widehat{x}, \widehat{p}] = \widehat{J}\,\hbar[\widehat{a}, \widehat{a}^\dagger] = \widehat{J}\,\hbar .$$

5.8 Physical Realization of Qubits

Recall that harmonic oscillator is *any* physical system with the Hamiltonian in the form

$$H = \frac{p^2}{2m} + \frac{kx^2}{2}\,.$$

Many physical systems can be described using this Hamiltonian and thus provide specific *realizations* of the oscillator model. Similarly, many concrete physical systems realize the idea of a qubit.

5.9 Interacting Qubits

Isolated quantum systems are idealizations. Interactions between systems are not only hard to avoid, but are often desirable for practical purposes. We now turn our attention to the interaction between a pair of simplest quantum systems – quantum qubits.

5.9.1 Joint State

Treating a pair of qubits as a single quantum system implies describing the state of two qubits with a single state vector $|\Psi\rangle$. It is called a *joint state* vector and is used to describe the results of measurements performed on a pair of qubits.

To measure two separate parts of a single quantum system one may use two detectors. Each detector measures a single qubit and finds it in either state $|0\rangle$ or $|1\rangle$ with different probabilities. The results of a *joint measurement* can be expressed as a linear combination of all possibilities:

$$|\Psi\rangle = c_{00}|0\rangle|0\rangle + c_{01}|0\rangle|1\rangle + c_{10}|1\rangle|0\rangle + c_{11}|1\rangle|1\rangle\,.$$

For example, if all results are equally probable, the state of the qubit-pair system can be written as follows:

$$|\Psi_0\rangle = \left(|0\rangle|0\rangle + |0\rangle|1\rangle + |1\rangle|0\rangle + |1\rangle|1\rangle\right)/2\,.$$

There are no *correlations* between the measurements for this state. Two qubits are not only spatially separated, but also *statistically unrelated*. In this case each qubit can be assigned its own state vector and the joint state $|\Psi\rangle$ is a product of two states:

$$|\Psi_0\rangle = |\psi\rangle|\phi\rangle$$

where $|\psi\rangle = (|0\rangle + |1\rangle)/\sqrt{2}$ and $|\phi\rangle = (|0\rangle + |1\rangle)/\sqrt{2}$.

Whenever the results from two detectors are correlated, the separation of a qubit pair into independent parts becomes impossible. The state $|\Psi\rangle$ then can't be factorized: $|\Psi\rangle \neq |\psi\rangle|\phi\rangle$. Indeed, suppose the state is

$$|\Psi_1\rangle = (|0\rangle|0\rangle + |1\rangle|1\rangle)/\sqrt{2}\,.$$

Assuming that $|\Psi\rangle = |\psi\rangle|\phi\rangle$ and $|\psi\rangle = a|0\rangle + b|1\rangle$ and $|\phi\rangle = c|0\rangle + d|1\rangle$, we get four requirements for the coefficients a, b, c and d:

$$\begin{aligned} ac &= 1/\sqrt{2}\,, & ad &= 0 \\ bd &= 1/\sqrt{2}\,, & bc &= 0\,. \end{aligned}$$

These requirements can't be satisfied, because a and d can't be zero, while their product must be zero (similarly b and c).

The state $|\Psi_1\rangle = (|0\rangle|0\rangle + |1\rangle|1\rangle)/\sqrt{2}$ is an example of *entangled* state of a qubit pair. It illustrates a peculiar quantum situation when the complete knowledge about the joint system does not mean complete knowledge of its "parts". In other words, in a strongly *correlated system* there are no independent parts which can be described with their own individual state vectors. Qubit pair acts as *one inseparable whole*.

Exercise 5.18

Suppose a qubit pair is in the state

$$|\Psi_2\rangle = (|0\rangle|1\rangle + |1\rangle|0\rangle)/\sqrt{2}\,.$$

Show that this state can't be written as the product state:

$$|\Psi_2\rangle \neq |\psi\rangle|\phi\rangle\,.$$

5.9.2 Computational Basis

The four joint states of a qubit pair

$$|\Upsilon_1\rangle = |0\rangle|0\rangle,\ |\Upsilon_2\rangle = |0\rangle|1\rangle,\ |\Upsilon_3\rangle = |1\rangle|0\rangle,\ |\Upsilon_4\rangle = |1\rangle|1\rangle$$

are called *computational basis*. It is often used in the field of quantum information processing. Each state of the computational basis has the

form of a product of states of separate qubits. State vectors of the computational basis are *not entangled*.

A general state of a qubit pair can be expanded in the computational basis:

$$|\Psi\rangle = \int c_i |\Upsilon_i\rangle \,.$$

A general operator representing processes involving qubit pair can also be written using computational basis:

$$\widehat{A} = \int a_{ij} |\Upsilon_i\rangle\langle\Upsilon_j| \,.$$

For example, transition operator describing the transfer of energy from the first qubit to the second takes the form $\widehat{T}_{12} = |\Upsilon_2\rangle\langle\Upsilon_3|$.

Exercise 5.19

Write general form of Hamiltonian of a qubit pair in the computational basis.

$$\widehat{H} = \int h_{ij} |\Upsilon_i\rangle\langle\Upsilon_j| \,.$$

Q: Are there other states, which are also basis and product? Smth like

$$|\Xi\rangle = |+\rangle|+\rangle \,.$$

5.9.3 Creating Entanglement

How do qubits become *entangled*? Let's show that an interaction between qubits, responsible for the transfer of energy from the first qubit to the second, can, in certain scenarios, lead to an entangled state. The mechanism described below is universal in the sense that it works for any two interacting quantum systems, not just a pair of qubits.

Energy exchange between two qubits implies the following transition:

$$|1\rangle|0\rangle \quad \longrightarrow \quad |0\rangle|1\rangle \,.$$

This is a process in which the first qubit is initially excited, and the second qubit is in the ground state, but in the end the first qubit drops into the ground state, while the second qubit becomes excited. Mathematically,

this transition is described by a product of operators:

$$\widehat{T}_{12}=\widehat{\sigma}_1 \otimes \widehat{\sigma}_2^+=\widehat{\sigma}_1\widehat{\sigma}_2^+ \ .$$

The qubits are identical and there is no fundamental reason for the energy to flow only in one direction. Therefore, the exchange must be reversible and described not only by $\widehat{T}_{12}$, but also by the opposite process:

$$\widehat{T}_{21}=\widehat{\sigma}_1^+ \otimes \widehat{\sigma}_2=\widehat{\sigma}_1^+\widehat{\sigma}_2 \ .$$

Hamiltonian with interaction between two qubits can then be written as follows:

$$\widehat{H}_\epsilon=\widehat{H}_1\widehat{I}_2 + \widehat{I}_1\widehat{H}_2 +\epsilon\left(\widehat{T}_{12} + \widehat{T}_{21}\right) , \tag{5.1}$$

where the parameter ϵ determines the strength of the interaction. Obviously, for $\epsilon = 0$ there is no interaction between the qubits.

Exercise 5.20
Show that the state $|\Psi_2\rangle = (|0\rangle|1\rangle + |1\rangle|0\rangle)/\sqrt{2}$ is the eigen-state of the Hamiltonian (5.1). Find the eigen-value (energy) for this state.
Suggestion: Use the fact that $E_1 = E_0 + \hbar\omega$.

Exercise 5.21
Check whether the state $|\Psi_3\rangle = (|0\rangle|1\rangle - |1\rangle|0\rangle)/\sqrt{2}$ is the eigen-state of the Hamiltonian (5.1).

Exercise 5.22
Find the result of the action of the Hamiltonian (5.1) on the state $|1\rangle|0\rangle$.

Now we can find how the state of the qubit pair changes from the initial $|1\rangle|0\rangle$ at time $t = 0$ to an entangled state a moment later. Schrödinger equation states

$$\partial_t|\Psi\rangle = -\frac{\widehat{J}}{\hbar}\ \widehat{H}_\epsilon\ |\Psi\rangle .$$

Therefore, after a time interval δt, the state evolves as

$$|\Psi\rangle \quad \longrightarrow \quad |\Psi\rangle + \delta|\Psi\rangle$$

where

$$\delta\,|\Psi\rangle = -\frac{\widehat{J}\,\delta t}{\hbar}\;\widehat{H}_\epsilon\;|\Psi\rangle\,.$$

For $|\Psi\rangle = |1\rangle|0\rangle$ the right-hand side becomes

$$\delta\,|\Psi\rangle = a|1\rangle|0\rangle + b|0\rangle|1\rangle\,,$$

where

$$a = -\,\widehat{J}\,(2E_0/\hbar + \omega)\delta t\,, \quad b = -\,\widehat{J}\,\epsilon/\hbar\delta t\,.$$

The key point is that due to the interaction term $\widehat{T}_{12}$ the initial state evolves into the superposition

$$|\Psi\rangle = (1+a)|1\rangle|0\rangle + b|0\rangle|1\rangle$$

which clearly has the form of an entangled state. Continuing this process, we will arrive, step by step, to a fully entangle state $|\Psi_2\rangle = (|0\rangle|1\rangle + |1\rangle|0\rangle)/\sqrt{2}$.

> ***Where is Energy?***
> When a qubit pair is entangled, neither qubit has definite energy. However, the system as a whole does have a certain energy. How is this energy "divided" between the qubits?

5.9.4 Bell States

Among the bases for a qubit pair some stand out due to their special properties. One such basis is named after John Steward Bell. The basis vectors can be expressed in terms of the computational basis as follows:

$$|\Phi^+\rangle = \frac{1}{\sqrt{2}}\,(|\Upsilon_1\rangle + |\Upsilon_4\rangle)\,, \tag{5.2}$$

$$|\Phi^-\rangle = \frac{1}{\sqrt{2}}\,(|\Upsilon_1\rangle - |\Upsilon_4\rangle)\,, \tag{5.3}$$

$$|\Psi^+\rangle = \frac{1}{\sqrt{2}}\,(|\Upsilon_2\rangle + |\Upsilon_3\rangle)\,, \tag{5.4}$$

$$|\Psi^-\rangle = \frac{1}{\sqrt{2}}\,(|\Upsilon_2\rangle - |\Upsilon_3\rangle)\,, \tag{5.5}$$

Each state vector of the Bell states basis corresponds to an entangled state. In fact, such states are *maximally entangled*, in contrast with the

computational basis.

Exercise 5.23
Express computational basis in terms of the Bell states.

Exercise 5.24
Express qubit pair Hamiltonian in terms of the operators built from Bell states.

5.9.5 GHZ State

The idea of entangled quantum systems can be naturally extended beyond a simple pair. If we are working with three qubits, their joint states can be written using a computational basis

$$|000\rangle, |001\rangle, |010\rangle, |011\rangle, |100\rangle, |101\rangle, |110\rangle, |111\rangle.$$

Each state from this basis is a product state and corresponds to a statistically independent (not entangled) states. Fully entangled states are possible, as one such state–GHZ state– is named after Daniel Greenberger, Michael Horne, and Anton Zeilinger. It has a simple form:

$$|GHZ\rangle = \frac{|000\rangle + |111\rangle}{\sqrt{2}}.$$

5.9.6 Qat States

Macroscopical systems, such as crystals, rocks, tables, animals, planets, and so on, contain an enormous number of "parts": molecules, atoms, protons and electrons. Such systems are extremely complex and their quantum description is challenging. However, researchers are constantly improving the techniques to create *macroscopic quantum states* – quantum states of systems with macroscopically large number of parts. Such quantum systems are sometimes called *macroscopic Schrödinger's cat states*. We will call them *qat states*.

Although a single biological cell does not exhibit quantum properties, let's model it as a qubit, with the states $|0\rangle$ and $|1\rangle$ representing a "dead" and "alive" cell, respectively. A body of a cat will have about $M = 10^{10}$ cells, and the state of M qubits can be written as a superposition of 2^M

computational basis vectors. Two extreme states have simple structure:

$$|A\rangle = |111\ldots1\rangle = |1\rangle^{\otimes M} \quad \text{– all cells are alive (alive cat),}$$

$$|D\rangle = |000\ldots0\rangle = |0\rangle^{\otimes M} \quad \text{– all cells are dead (dead cat).}$$

Exercise 5.25

What does the following state correspond to:

$$|B\rangle = |0111\ldots1\rangle\,?$$

How many cells need to be "alive" for the cat to be considered alive?

The following qat state is very interesting:

$$|S\rangle = \frac{|A\rangle + |D\rangle}{\sqrt{2}}\,.$$

Dead or Alive?

Erwin Schrödinger first discussed such a state in his 1935 paper XXX, using a cat as an example. Today the term "Schrödinger's cat" is one of the most recognized expressions from quantum physics. What is not usually mentioned, is the purpose of Schrödinger's example.

5.10 Quantum Field

We are looking for a binary operator $\widehat{\sigma}$ that yields a number based on two vectors:

$$|\sigma\rangle\langle\sigma|\,\vec{a}\,\vec{b} = x\,.$$

We are looking for a binary operator $\widehat{\sigma}$ that yields a number based on two vectors:

$$\widehat{\sigma}\;\vec{a}\,\vec{b} = x\,.$$

We will call this operator $\widehat{\sigma}$ *dol*-operator[1], based on the key letters of the phrase "degree of overlap".

[1] This is not a standard terminology.

Reminder
When we say that an operator $\widehat{\Gamma}$ is given or known, we mean that we know how it acts on *any vector* $\vec{a}$:

$$\widehat{\Gamma}\ \vec{a} = x_a\,.$$

Array of equations:

$$\widehat{\Gamma}_1\ \vec{e}_1 = 1 \tag{5.6}$$
$$\widehat{\Gamma}_1\ \vec{e}_2 = 0 \tag{5.7}$$
$$\widehat{\Gamma}_1\ \vec{e}_3 = 0 \tag{5.8}$$
$$\ldots \tag{5.9}$$

5.11 Quantum States of Light Chapter Highlights

- *Two vectors can be compared for similarity by calculating the "degree of overlap". The longer two vectors are and the closer their mutual direction – the greater the overlap is.*
- *Degree of overlap can be described by a binary linear operator* $\widehat{\sigma}$*. This operator is closely related to the concept of scalar product of two vectors.*
- *When scalar product (or, equivalently, degree of overlap) is defined for vectors, each vector receives a "special relative" – conjugate vector – that lives in different vector space, called conjugate or dual space.*
- *When the degree-of-overlap operator* $\widehat{\sigma}$ *is partially applied, the result is a unary linear operator that yields a number for every input vector. Importantly, such an operator is also a vector, albeit not an arrow-like vector.*

6. Applications

We are now ready to appreciate how tensors are used in "real life". In this chapter we will encounter examples of tensors that are used in mathematics, physics, and engineering.

> ☑ ***Prerequisite Knowledge***
> To fully understand the material of this chapter, readers should be comfortable with the following concepts:
> - State
> - Dynamical equations

6.1 Hydrogen-like Atoms

We will start with the simplest atomic system: Hydrogen atom.

6.1.1 Hydrogen Atom

The most abundant element in the observable universe is hydrogen. A hydrogen atom has two components: heavy nucleus (proton) and light "shell" (electron). The two components can be separated in the process of *ionization*. A significant energy is required to tear-off the shell:

$$E_{ion} = 2.18 \times 10^{-18} (J) = 13.6 \, (eV) \, .$$

These numbers do not look big; however, they correspond to an extremely high temperature:

$$T_{ion} = \frac{E_{ion}}{k} = \frac{2.18 \times 10^{-18}}{1.38 \times 10^{-23}} = 157\,887 \, (K) \, .$$

This is almost 30 times higher than the temperature near the "surface" of the sun; the estimated temperature in the core of the sun is about 100 times higher than the hydrogen ionization temperature.

The bottomline is that in normal conditions the electron is reliably *trapped/localized/confined* in a small region near the nucleus. The diameter of hydrogen atom provides a convenient "scale" for distances in atomic world:

$$d_H \approx 1\,\text{Å} \qquad \text{Ångstrom } = 10^{-10}\,(m)\,.$$

⊛ Illustration

If every person on earth had a hydrogen atom and placed it in a single row next to each other, then the resulting chain would be about a meter long.

Ångstrom

Angstrom is a convenient unit for measuring distances between atoms inside solid bodies. For example, copper atoms are about 2.8 Å in diameter and are arranged in a crystal with the distance between the nearest neighbors $d \approx 3.6$ Å.

To see how those values for the ionization energy and atomic radius appear, let us consider the following model of the atom, shown in the Figure 6.1.

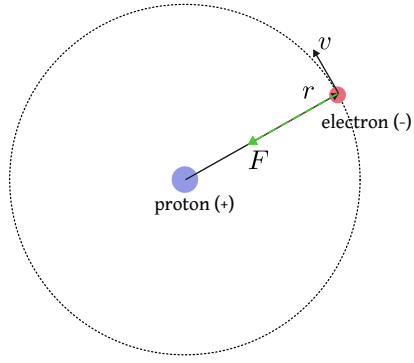


Fig. 6.1: Planetary model of hydrogen atom.

The circular motion of the electron around the nucleus is mathemati-

cally similar to the problem of a planet circling a star. Using the second law of Newton and the expression for the Coulomb's force, we can write

$$\frac{m_e v^2}{r} = k\frac{q_e^2}{r^2}\,,$$

where

$$k = \frac{1}{4\pi\varepsilon_0}\,.$$

Newtonian momentum is given by $p = mv$; from the motion equation above, we find

$$p^2 = k\frac{m_e q_e^2}{r}\,.$$

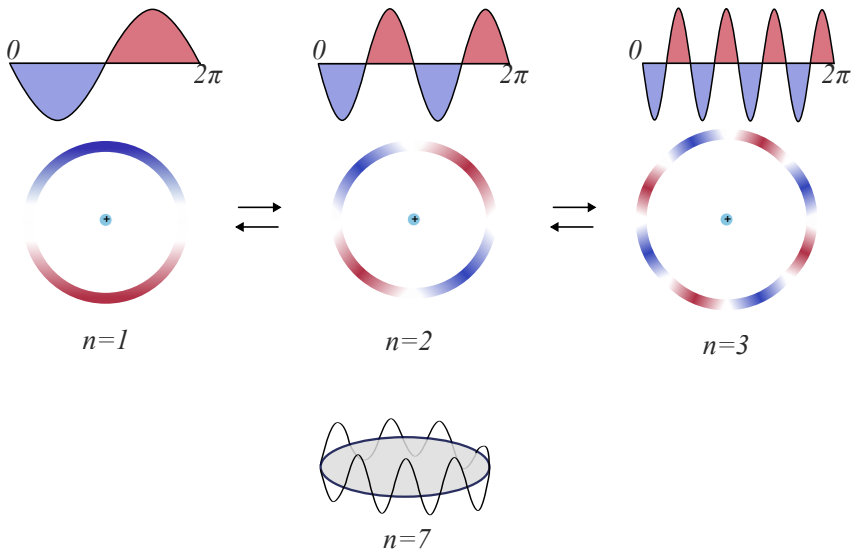


Fig. 6.2: Orbits allowed by the semi-quantum model.

Using de Broglie hypothesis about the relation between momentum and wavelength

$$p\lambda = h\,,$$

and combining it with *quantization hypothesis*:

$$n\lambda = 2\pi r$$

or, equivalently,

$$pr = n\frac{h}{2\pi} = n\hbar$$

we find possible solutions for the radius of the "orbit":

$$r_n = \frac{\hbar^2 n^2}{k m_e q_e^2} \qquad n = 1, 2, 3, \ldots$$

The smallest value of the radius is

$$a_0 = r_1 = \frac{4\pi\varepsilon_0 \hbar^2}{m_e q_e^2} = 0.523\,\text{Å}\,.$$

It is called *Bohr radius*. Thus, the smallest diameter of electron's orbit is about 1 Ångstrom.

Exercise 6.1
Find the numbers for which the radius of electron "orbit" equals: 1) 1 mm; 2) 1 cm; 3) 1 m.

How fast does the electron move around the nucleus? The velocity of the electron is

$$v = \sqrt{\frac{k q_e^2}{m_e r}}\,.$$

Substituting $r_n = a_0 n^2$ we get

$$v_n = \frac{1}{n}\sqrt{\frac{k q_e^2}{m_e a_0}} = \frac{v_1}{n}\,.$$

The value of v_1 is

$$v_1 = 2.19 \times 10^6\,(m/s)$$

Although this is a big number, it is much smaller than the speed of light; we are therefore justified in using Newtonian mechanics and not taking relativity into account.

⊛ Fun Fact

The "quantization" of orbit radius can be found even for planets in solar system. If we denote the distance between the earth and the sun as A (called *astronomical unit*), then the distances to planets from the sun are given by the formula

$$r_n = \frac{A}{10}(4 + 3 \times 2^n) .$$

This relation is known as *Titius-Bode* law. It works remarkably well for all planets from Venus ($n = 0$) to Uranus ($n = 6$).

How strong is the electron attracted to the nucleus? The Coulomb force between the charges is

$$F = \frac{kq_e^2}{r^2} .$$

Substituting $r_n = a_0 n^2$ we get

$$F_n = \frac{kq_e^2}{a_0^2 n^4} = \frac{F_1}{n^4} .$$

The value of F_1 is

$$F_1 = 8.24 \times 10^{-8} \, (N)$$

This is a tiny force on the human scale of forces.

⊛ Fun Fact

Even a baby ant has enough force to tear a hydrogen atom apart with its bare hands!

Although the force acting on the electron is small on a human scale, the acceleration ($a = v^2/r$) it produces is very large (on the human scale, compare to g). This is due to extreme lightness of the electron:

$$m_e = 9.1 \times 10^{-31} \, (kg) .$$

What is the total energy of the hydrogen atom? It can be found as

follows:

$$E_n = \frac{m_e v_n^2}{2} - k\frac{q_e^2}{r_n} = -\frac{E_1}{n^2},$$

where

$$E_1 = k\frac{q_e^2}{2m_e a_0}.$$

The value of E_1 is

$$E_1 = 2.18 \times 10^{-18}\,(J).$$

In atomic world a special unit of energy is used. It is the energy of electon accelerated by a voltage drop of 1 Volt:

$$E_{ev} = 1\,(V) \times q_e = 1.6 \times 10^{-19}\,(J).$$

Using this atomic unit, the hydrogen atom has energy

$$E_1 = 13.6\,(eV).$$

Exercise 6.2
What is the frequency of revolution of electron around the nucleus for an orbit number n?

Atoms Can't Exist?

The model described above leads to the conclusion that atoms must not exist for long. According to the theory of classical electrodynamics, a charge moving in a circle will emit electromagnetic waves with the frequency of revolution. As the atom loses its energy, the electron spirals ever closer to the nucleus. Taking classical electrodynamics into account, the life-time of a hydrogen atoms should be about nanosecond. This contradicts the observation of stability of atoms.

Niels Bohr suggested that the "orbits" represent so called *stationary states*, where electrons can "move" without radiating away electromagnetic waves. Radiation only happens when electron *transitions* between stationary levels, for example between 2 and 4. The energy carried away by the light is related to the frequency of the electromagnetic wave ν as follows:

$$\Delta E = E_m - E_n = h\nu_{nm} \qquad m > n.$$

Exercise 6.3
How much energy is required to "move" electron from the"orbit" of 1 mm to 1 cm? From 1 cm to 1m?

Line Spectra Explained

Using the results obtained above, we can now describe the spectra of light emitted or absorbed by hydrogen.

The stationary states are discrete, therefore there are discrete energies of transition between a pair of levels. When atom absorbs electromagnetic radiation, electron "jumps up" to higher energy level and farther distance. In the reverse process, electron "jumps down" from higher level to lower one, resulting in emission.

The wavelength of the radiation is

$$\lambda = cT = \frac{c}{\nu} = \frac{ch}{E_m - E_n}.$$

Plugging in the expression for the energy, we get

$$\lambda = \frac{ch}{E_1}\frac{n^2m^2}{m^2 - n^2} = 91.127(nm) \times \frac{n^2m^2}{m^2 - n^2}. \tag{6.1}$$

A special case of this formula was discovered in 1885 by a Swiss mathematician Johan Balmer. Analyzing the visible lines in the spectra of hydrogen, he found some regularity in the wavelengths. Balmer expressed it as follows:

$$\lambda = B\frac{m^2}{m^2 - 2^2},$$

where $m > 2$ and $B = 364.51$ nm. Looking at (6.1), we can see that it can be written for $n = 2$ as

$$\lambda = 91.127(nm) \times \frac{4m^2}{m^2 - 2^2} = 364.51(nm) \times \frac{m^2}{m^2 - 2^2}.$$

Exercise 6.4
According to the the formula (6.1), how many hydrogen lines will be in the visible part of the spectrum (from 400nm to 700nm)?

> ***Three Body Problem***
> The problem of hydrogen atom involves *three* physical entities interacting with each other: Proton, electron, and electromagnetic field. Electron does not interact directly with the proton, it does so via the electric field of the nucleus. This is important to keep in mind, especially if we want to understand the phenomenon of *spontaneous emission*.

Spontaneous Emission and Cavity QED

According to Schrodinger equation, an hydrogen atom with electron in any statioary state $|\Psi_n\rangle$ with energy E_n will remain in this state *forever*. In reality, every atom will randomly transition into a state with lower energy, all the way to the lowest energy state, emitting radiation as the result. This is called *spontaneous emission*.

To describe spontaneous emission, one must account for the fact that atom is not truly isolated and electron and proton are not the only quantum systems in picture. There is an electromagnetic field with its many modes-oscillators.

Interaction of atom-like quantum systems (qubits, quantum dots, atoms) with quantum states of electromagnetic field is the focus of an exctiting area of research called *Cavity Quantum Electrodynamics* or *cavity QED*.

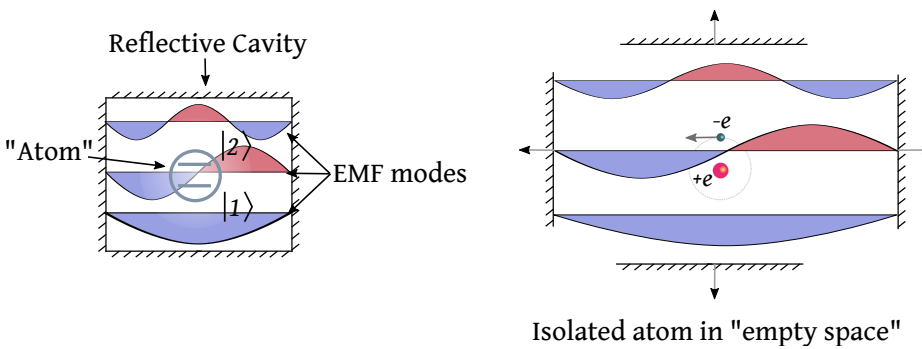


Fig. 6.3: Atom in “empty space” is a quantum system in a very large cavity, coupled to the modes-oscillators of electromagnetic field.

6.1.2 Franck-Hertz Experiment

Atoms can transition between different states by absorbing energy from electromagnetic radiation ("photons"). But this is not the only mechanism. Other particles, like electrons, can transfer their kinetic energy to atoms by bumping into the latter. Such a phenomenon was studied by James Franck and Gustav Hertz in 1914 using collisions of electrons with mercury atoms enclosed in a special vacuum tube. They showed that whenever electrons had a certain kinetic energy – specific to mercury atoms – they transfered this energy very efficiently (*resonantly*) to mercury atoms. When the energies of electrons and mercury atoms were not matched, electrons scattered from the atoms *elastically* – without the loss of their kinetic energy. The work of Franck and Hertz was recognized with 1925 Nobel Prize in Physics. Interestingly, according to James Franck, neither he nor Gustav Hertz had any knowledge of Bohr's theory of atomic states when they performed their experiment.

Idea

The idea of Franck-Hertz experiment is illustrated in figure 6.4. Its central part consists of a closed vacuum tube with mercury gas and several electric elements used as the source and sink of electrons.

Numbers

At room temperature mercury is a liquid metal which can be easily turned into a gas by heating it up to 200°C. Unlike molecular gases such as hydrogen H_2, oxygen O_2, or nitrogen N_2, *mercury gas is monoatomic* – consisting of single Hg atoms.

Each mercury atom contains 80 protons and 120 neutrons and is significantly heavier than an electron: $M_{Hg} \approx 4 \times 10^5\, m_e$. Consequently, an electron colliding with a mercury atom won't be able to impart any appreciable recoil speed. In other words, mercury atoms are like immovable objects to electrons.

Exercise 6.5
Show that for the head-on collision the speed of an initially stationary mercury atom after the collision becomes $v = 2v_0 \frac{m_e}{M_{Hg}}$.

6.1.3 Stoke's Rule

Stoke's rule.

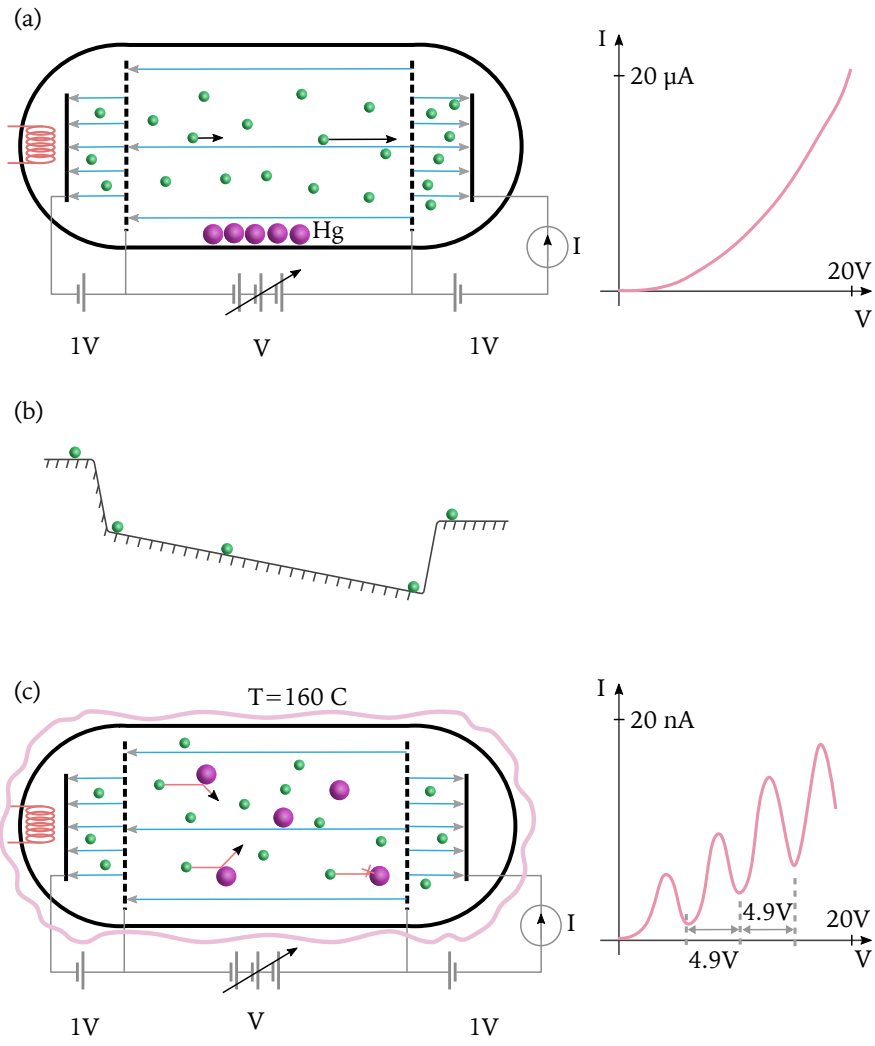


Fig. 6.4: (a) A vacuum tube is used to study the flow of electrons between two metal electrods under various conditions.; (b); (c).

6.2 Rydberg Atoms

When an atom has outer electron(s) excited into states with high excitation number n, it is called a *Rydberg atom*(CHECK!). Such atoms are of great importance for experiments of quantum physics.

6.3 Quantum Dots

Quantum dots can be viewed as *artificial atoms* – human-made physical structures designed to confine electrons in tiny volumes. As the result, quantum states of the trapped electrons form a discrete set not unlike the states of a hydrogen atom. *Examples:???*

To illustrate the idea, consider an idealized case of an electron confined in one dimension in a region between $x = 0$ and $x = L$.

$$|\alpha\rangle\langle\beta|$$

$$E_n = -\frac{E_i}{n^2}\,.$$

6.4 Spontaneous Emission

$$|\alpha\rangle\langle\beta|$$

$$E_n = -\frac{E_i}{n^2}\,.$$

6.5 Stimulated Emission

$$|\alpha\rangle\langle\beta|$$

$$E_n = -\frac{E_i}{n^2}\,.$$

6.6 Lasers

From the standpoint of quantum physics, lasers are special *sources of excitation of electromagnetic field.* Laser's operation is based on the effect of **L**ight **A**mplification by the **S**timulated **E**mission of **R**adiation (LASER).

$$|\alpha\rangle\langle\beta|$$

$$E_n = -\frac{E_i}{n^2}\,.$$

6.7 Photoeffect

$$|\alpha\rangle\langle\beta|$$

$$E_n = -\frac{E_i}{n^2}\,.$$

6.8 Black Body Radiation

$$\rho_\nu = \frac{2h\nu^3}{c^2}\frac{1}{e^{h\nu/kT}-1}\,.$$

$$E_n = -\frac{E_i}{n^2}\,.$$

6.9 Conductors

$$|\alpha\rangle\langle\beta|$$

$$E_n = -\frac{E_i}{n^2}\,.$$

6.9.1 Heat Capacity

Einstein's model.

6.10 Entanglement

Entanglement can be viewed as a *physical resource* of purely quantum nature. As a resource, entanglement facilitates several important processes related to processing of information.

$$|\alpha\rangle\langle\beta|$$

$$E_n = -\frac{E_i}{n^2}\,.$$

6.10.1 Teleportation

In quantum physics *teleportation* means instant creation of a desired quantum state at a far away place. It important to understand that quantum teleportation does not imply sending objects or energy instanteneously from one place to another.

6.10.2 Entanglement And Measurement

δ-Notation

When a quantity x changes by a tiny amount, we will denote the change using small Greek letter δ (delta) as follows:

$$\boxed{\delta x \text{ - tiny change of } x.}$$

A convenient way to write all components of a second rank tensor is to use table-like structure called *matrix*:

$$F^{\mu\nu} = \begin{pmatrix} F^{00} & F^{01} & F^{02} & F^{03} \\ F^{10} & F^{11} & F^{12} & F^{13} \\ F^{20} & F^{21} & F^{22} & F^{23} \\ F^{30} & F^{31} & F^{32} & F^{33} \end{pmatrix}.$$

In the matrix, the first index μ of $F^{\mu\nu}$ corresponds to the row, while the second index ν corresponds to the column. Both rows and columns are enumerated from 0 to 3.

Using matrix form, we can write the electromagnetic tensor in terms of the electric and magnetic fields:

$$F^{\mu\nu} = \begin{pmatrix} 0 & -\mathcal{E}^1 & -\mathcal{E}^2 & -\mathcal{E}^3 \\ \mathcal{E}^1 & 0 & -\mathcal{B}^3 & \mathcal{B}^2 \\ \mathcal{E}^2 & \mathcal{B}^3 & 0 & -\mathcal{B}^1 \\ \mathcal{E}^3 & -\mathcal{B}^2 & \mathcal{B}^1 & 0 \end{pmatrix}.$$

Chapter Highlights

- *Tensors find application in various areas of science and math.*
- *Geometrical properties of surfaces and spaces can be described using metric tensor.*
- *Physical properties of solids are often anisotropic – depend on the direction of applied "force". Such properties are best described by various tensors: stress tensor, mobility tensor, piezoelectric tensor, and others.*
- *At the fundamental level electric and magnetic fields are united in a*

single physical object – electromagnetic field. Electromagnetic field is described by an antisymmetric tensor of the second rank.

7. Implications

We are now ready to appreciate the implications of quantum physics.

> ☑ ***Prerequisite Knowledge***
> To fully understand the material of this chapter, readers should be comfortable with the following concepts:
> - State
> - Dynamical equations

Discuss Mermins papers. Wheeler's ideas.

δ-Notation
When a quantity x changes by a tiny amount, we will denote the change using small Greek letter δ (delta) as follows:

$$\boxed{\delta x \text{ - tiny change of } x.}$$

A convenient way to write all components of a second rank tensor is to use table-like structure called *matrix*.

Chapter Highlights

- *Tensors find application in various areas of science and math.*
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8. Appendix

We are now ready to appreciate the implications of quantum physics.

8.1 Physics

When a quantity x changes by a tiny amount, we will denote the change using small Greek letter δ (delta) as follows:

δx - tiny change of x.

A convenient way to write all components of a second rank tensor is to use table-like structure called *matrix*.

8.1.1 Black Body Radiation

8.1.2 Notation

K and E_k – Kinetic energy of a system.
Π and E_p – Potential energy of a system.
E – Total mechanical energy ($E = E_K + E_P$) written in terms of velocity v and position x.
H – Hamiltonian of a system: $H = K + \Pi$. Differs from E because kinetic energy written in terms of *momentum* p instead of velocity.
L – Lagrangian (Lagrange function) of a system: $L = E_K - E_p$. It is the "imbalance" of energies.
Δx – Change of a value of a variable x.
δx – "Tiny" change of a value of a variable x.
∂ – Rate of change.
∂_t – Rate of change with respect to time.
∂_x – Rate of change with respect to variable x (e.g. position).
$\partial_t f$ – Rate of change of f with respect to t.

It means exactly the following

$$\partial_t f = \frac{\delta f}{\delta t} = \frac{f(t+\delta t) - f(t)}{\delta t}\,.$$

$\vec{\xi}$ – State of a system in Hamiltonian dynamics. It is a vector with components $\vec{\xi} = (x, p)$.
$\hat{J}$– Operation (operator) of rotation by 90 degrees.
$\hat{R}(\theta)$ – Operation (operator) of rotation by θ.
h – Quantum of action (Planck's constant). In SI units its numerical value is $h = 6.626 \times 10^{-34}(J \cdot s)$.
$\hbar$ – "Reduced Planck's constant". A convenience notation for often used combination $\hbar = h/(2\pi)$.
A – Action.
Ψ – Quantum state.
$|\Psi\rangle$ – Quantum state vector.
ϕ, θ – Angle variables.
ω – Angular speed (also angular velocity). Often it has the following meaning: $\omega = \partial_t \theta$.
$\vec{e_1}, \vec{e_2}$ – Basis vectors. Usually they have unit length and point in mutually perpendicular directions.
z – Arbitrary *numeric* variable, $\vec{z}$ – arbitrary *vector* variable, $\hat{z}$ – arbitrary *operator*.
$\mathring{A}$ – Angstrom, a unit of length in the world of atoms. $1\mathring{A} = 10^{-9}(m)$. Hydrogen atom is about $1\mathring{A}$ in diameter.
c – Speed of light in vacuum.
ν – Frequency of oscillations measured as the number of oscillations per second, in Hz.

8.1.3 Physical Constants

Below is the list of various physical constants used in these notes.
$q_e = 1.6 \times 10^{-19}\,(C)$ – Charge quantum (charge of an electron).
$m_e = 9.1 \times 10^{-31}\,(kg)$ – rest-energy (aka mass) of an electron.
$k = \frac{1}{4\pi\epsilon_0} = 9 \times 10^9\,(N \cdot m^2/C^2)$ – Coulomb constant – force between two unit charges 1 meter apart.
10^{-9} s = 1 nanosecond – the unit of time in atomic world. It is a "heartbeat of atoms".
$1\,(eV) = q_e\,(J)$ – 1 electron-volt. It is the kinetic energy an electron

would acquire when accelerated by a simply 1V battery. A tiny value.
$m_e c^2/q_e = 0.5\,MeV$ – rest-energy of an electron measured in electron-volts. Roughly speaking, we will need half a million 1-volt batteries to accelerate an electron to make its kinetic energy comparable to its rest-energy.
$k = 100\,(N/m)$ is a spring constant of a spring that stretches by 0.1 of a meter when 1 kilogram mass is attached to it.

8.2 Mathematics

When a quantity x changes by a tiny amount, we will denote the change using small Greek letter δ (delta) as follows:

δx - tiny change of x.

A convenient way to write all components of a second rank tensor is to use table-like structure called *matrix*.

8.2.1 Greek Alphabet

A α	alpha	B β	beta
Γ γ	gamma	Δ δ	delta
E ϵ	epsilon	Z ζ	zeta
H η	eta	Θ θ	theta
I ι	iota	K κ	kappa
Λ λ	lambda	M μ	mu
N ν	nu	Ξ ξ	xi
O o	omicron	Π π	pi
P ρ	rho	Σ σ	sigma
T τ	tau	Υ υ	upsilon
Φ ϕ	phi	X χ	chi
Ψ ψ	psi	Ω ω	omega

Table 8.1: Greek Alphabet

In mathematics most often we use θ and ϕ for angles. Sometimes α and β are also used. Occasionally ψ is used to denote angle.

In physics λ is used to denote the wavelength of light, ν – frequency in Hertz (periods of oscillations per second), ω – angular speed (number

of radians of rotation per second).

The symbols Ψ and Φ are usually used to denote quantum state vectors.

8.2.2 Available Environments

Coloredboxed environment, with \coloredboxed{color}{ text }:

$$\boxed{E = mc^2}.$$

Bold text command inside math mode is \btc{ txt}:

$$\mathbf{max}\, x\, y$$

Bold text with emphasis (italic) is done with \bem{text}: ***example of a very important piece of text***.

Grey bullet: \tus: • • • •

Quantum state is \qs: $|\psi\rangle$ or better use ket and bra commands: $|\phi\rangle$ and $\langle\psi|$.

Bracket and ketbra combinations using a single command: $\langle\psi|\phi\rangle$ and $|\psi\rangle\langle\phi|$.

Operators are set with \op{name}: $\widehat{\rho}= |\psi\rangle\langle\psi|$.

$$\hat{\rho} \neq \widehat{\rho}$$

Environments

Prerequisite environment \myprereq{text}:

☑ ***Prerequisites***
One, two, and three.

Example environment \myExample{text}:

💬 ***Example***
This is a perfect example.

Analogy environment \analogy{text}:

☼ ***Analogy***
Consider the following analogy: A and B.

Definition environment \mydef{text}:

Definition 8.1 *Kinetic Energy*
Kinetic energy is the energy due to motion.

Reminder environment \myrem{text}:

Kinetic Energy
Recall that $E_k = mv^2/2$.

Bio environment \mybio{text}:

Max Planck
The full name of Max Planck is Max Karl Ernst Ludwig Planck.

8.3 Temporary Stuff

Work in progress sections will be kep here.

8.3.1 Facts About Light

Our understanding of the physical nature of light is the result of several centuries of studies. Visible, infra-red or ultra-violet light, and microwave or gamma radiation are all various manifestations of *electro-magnetic field* (EMF). It is one of the most technologically important and well-understood fields.

Omnipresence

The first important fact about EMF is that it is truly ubiqutous: There is no place in the universe free from EMF. Yes, there are regions of space (and time) where EMF is not excited, but EMF is still present there in its "unexcited" form, called *EMF-vacuum*. This vacuum state is an important quantum state of EMF. It is discussed in more details in Section XXX.

Localizability

The second important fact about EMF is its ability to be localized (concentrated) in finite regions of space, simetimes in small volumes. Put differently, EMF can be excited ("emitted") by relatively small "objects" (sources of EMF excitations) or absorbed by similar objects. Emission and absorption of light by atoms is a perfect example of this principle.

> ***Localized Excitations***
> We must clarify: It is the *excitation of EMF* which is localized, *not* EMF. The latter is everywhere, always.

Energy-Momentum

Excitations of EMF propagate through space and possess the basic mechanical aspect – *energy-momentum*. When an atom emits a pulse of light it loses certain energy when and it also experiences a recoil, like a gun that fires a bullet. An EMF excitation carrying energy E also carries momentum p. The two are related as follows:

$$E = pc\,,$$

where c is the speed of light – the speed of propagation of EMF through "empy" space. This formula is a special case of a more general relation between energy and momentum, derived in the special theory of relativity:

$$E^2 = p^2c^2 + m^2c^4\,.$$

This is the relation between *total* (kinetic and non-kinetic) energy of an object with mass m and momentum p. It shows that even for an object at rest ($p = 0$) it still possesses non-kinetic energy – called rest-energy – equal $E_0 = mc^2$. For EMF excitations the total energy E is *purely due to motion* or, equivalently, EMF excitations are massless $m = 0$.

> ***Photons***
> In common language, propagating EMF excitations are called *photons*. It is sometimes said that photons with energy E carry momentum $p = E/c$ and that photons are massless particles. It must be emphasized again that such language is not always helpful.

Colors

Beyond energy-momentum, EMF excitations exhibit various "colors" – both visible and invisible to the human eye.

Timeless Law

The laws that describe the behavior of electromagnetic radition in space and time are expressed by the equations which show no preference to the direction of time flow.

9. Solutions

Exercise 1.1

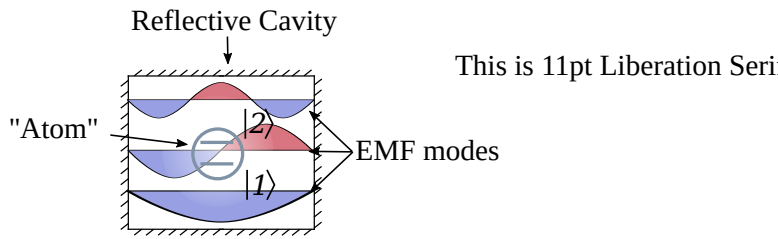

Fig. 9.1: The set M contains all possible makes of cars: Ford, Toyota, etc.

The diagram in the Figure 9.1 shows the set M – the set of all possible makes of cars. A mapping **trk** returns $true$ if a given car maker produces trucks.

Exercise 2.1

Any binary function can be viewed as a unary function if two inputs are replaced by a single input of a *pair of numbers*. Similarly for a function with two outputs. This idea is illustrated in the Figure 9.2(a): The function **swp** is viewed as a unary function which swaps the numbers in an *ordered pair*:

$$\textbf{swp}\ (n, m) = (m, n)\,.$$

Given the set $\mathbb{Z}$ of whole numbers, we can create the set of all possible *ordered pairs* (n, m). This set can be denoted as follows:

$$(\mathbb{Z}, \mathbb{Z})\ \text{ or }\ \mathbb{Z} \times \mathbb{Z}\,.$$

The latter notation is standard in mathematics, but the former way of writing is

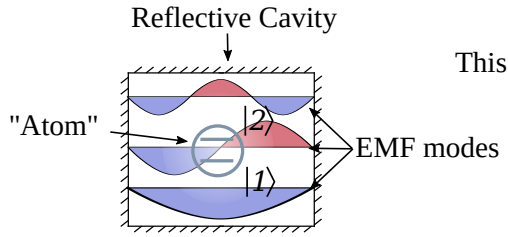

Fig. 9.2: (a) Two inputs (outputs) of a function can be replaced with a single input of a ***pair*** of numbers, turning a binary function into a unary one. (b) That.

also acceptable. We can similarly denote the set of all *ordered triples*:

$$(\mathbb{Z}, \mathbb{Z}, \mathbb{Z}) \text{ or } \mathbb{Z} \times \mathbb{Z} \times \mathbb{Z}\,.$$

With the notation introduced above, the action of functions with multiple inputs or outputs can be depicted on the level of sets. The Figure 9.2(b) shows how this works for the functions **swp** and **max** .

Index