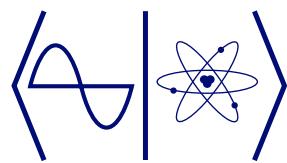


# EXPLORATIONS IN QUANTUM PHYSICS

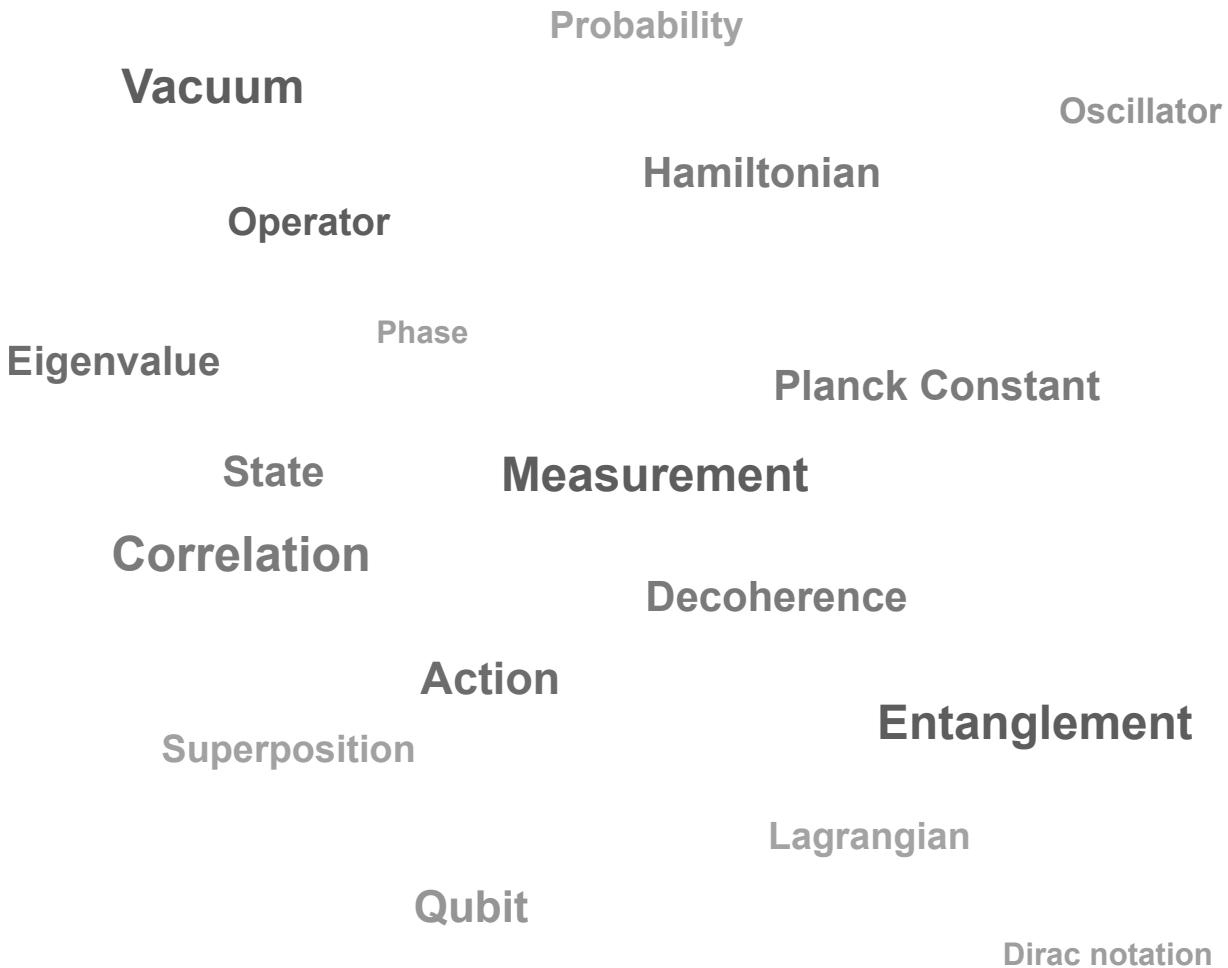


COURSE BOOK

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 COLUMBIA UNIVERSITY  
IN THE CITY OF NEW YORK

2024



# 2024

| July |     |     |     |     |     |     | August |     |     |     |     |     |     |
|------|-----|-----|-----|-----|-----|-----|--------|-----|-----|-----|-----|-----|-----|
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TEST DAY

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## Learning Progress Tracker

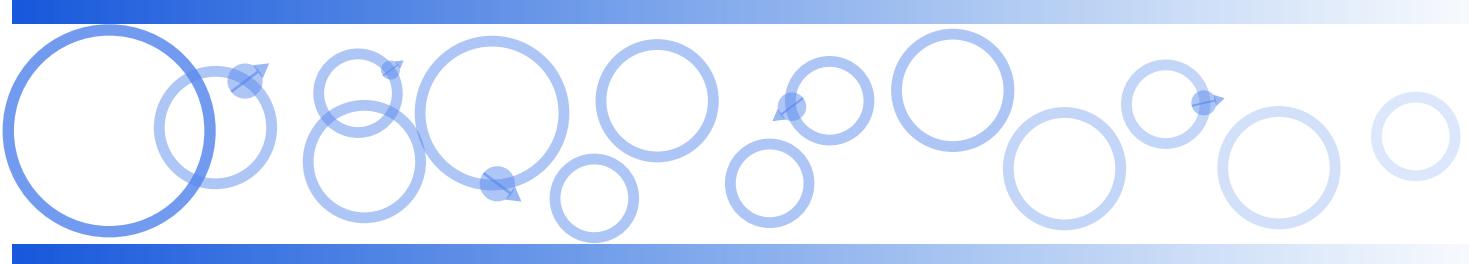
Students will check the boxes as they learn corresponding material. A good progress is achieved when at least 15 boxes are checked.

### Core

- Understand the fundamental concepts of *system* and *state*.
- Understand the idea of *state evolution* and *dynamical equations*.
- Become familiar with the method of *phase space*.
- Become familiar with the concepts of *Hamiltonian* and *Lagrangian*.
- Become proficient with *complex numbers*.
- Understand the meaning of *Hamiltonian equations*.
- Understand the idea of a *linear operator*.
- Become familiar with the method of *configuration space*.
- Understand the concept of *action* and the meaning of *Least Action Principle*
- Can write down Hamiltonian and Lagrangian for a *classical oscillator*.
- Can write down and interpret *Schrödinger equation*.
- Understand the importance of *measurement apparatus* in quantum physics.
- Can write down Hamiltonian for a *quantum oscillator*.
- Can write down Hamiltonian for a *qubit*.
- Understand the idea of *quantum vacuum*.
- Understand the concept of *entanglement*.

### Extra

- Be able to find components of a linear operator.
- Apply quantization of action to hydrogen atom to find states.
- Apply the principle of stationary action to a simple system.
- Define *local realism*.



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## Greek Alphabet

|                   |         |                     |         |
|-------------------|---------|---------------------|---------|
| A $\alpha$        | alpha   | B $\beta$           | beta    |
| $\Gamma \gamma$   | gamma   | $\Delta \delta$     | delta   |
| E $\epsilon$      | epsilon | Z $\zeta$           | zeta    |
| H $\eta$          | eta     | $\Theta \theta$     | theta   |
| I $\iota$         | iota    | K $\kappa$          | kappa   |
| $\Lambda \lambda$ | lambda  | M $\mu$             | mu      |
| N $\nu$           | nu      | $\Xi \xi$           | xi      |
| O o               | omicron | $\Pi \pi$           | pi      |
| P $\rho$          | rho     | $\Sigma \sigma$     | sigma   |
| T $\tau$          | tau     | $\Upsilon \upsilon$ | upsilon |
| $\Phi \phi$       | phi     | X $\chi$            | chi     |
| $\Psi \psi$       | psi     | $\Omega \omega$     | omega   |

Table 1: Greek Alphabet

In mathematics most often we use  $\theta$  and  $\phi$  for angles. Sometimes  $\alpha$  and  $\beta$  are also used. Occasionally  $\psi$  is used to denote angle.

In physics  $\lambda$  is used to denote the wavelength of light,  $\nu$  – frequency in Hertz (periods of oscillations per second),  $\omega$  – angular speed (number of radians of rotation per second).

The symbols  $\Psi$  and  $\Phi$  are usually used to denote quantum state vectors.

## Notation Used In Course

$K$  and  $E_k$  – Kinetic energy of a system.

$\Pi$  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.

$\Delta x$  – Change of a value of a variable  $x$ .

$\delta x$  – “Tiny” change of a value of a variable  $x$ .

$\partial$  – Rate of change.

$\partial_t$  – Rate of change with respect to time.

$\partial_x$  – 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  $\theta$ .

$h$  – 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.

$\Psi$  – Quantum state.

$|\Psi\rangle$  – Quantum state vector.

$\phi, \theta$  – Angle variables.

$\omega$  – 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*.

$\text{\AA}$  – Angstrom, a unit of length in the world of atoms.  $1\text{\AA} = 10^{-9}(m)$ . Hydrogen atom is about  $1\text{\AA}$  in diameter.

$c$  – Speed of light in vacuum.

$\nu$  – Frequency of oscillations measured as the number of oscillations per second, in Hz.

## Numerical Values

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.

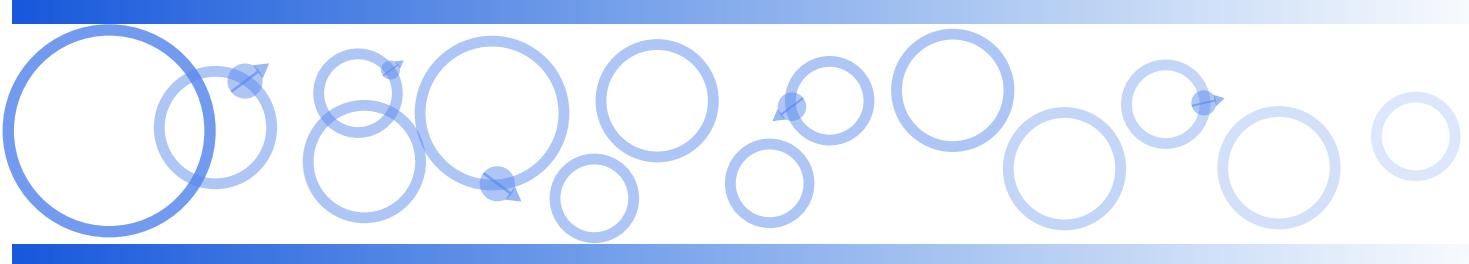
$k = \frac{1}{4\pi\epsilon_0} = 9 \times 10^9 (N \cdot m^2/C^2)$  – Coulomb constant – force between two unit charges 1 meter apart.

$10^{-9} \text{ s} = 1 \text{ nanosecond}$  – 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.

$m_e c^2/q_e = 0.5 \text{ MeV}$  – 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.



# DISCLAIMER

These notes are NOT complete and contain numerous typos and errors. The notes contain main results and ideas that will be covered during the course. They will be supplemented by additional print-outs.

Note that the line spacing in the course book is enlarged. You are encouraged to leave comments/notes/marks on the pages and provide feedback to the instructor.

## Keys To Success

The course is very intense and sometimes unevenly paced. To maximize its effect it is very important to stay engaged. Try to focus on the course and don't get distracted by other activities. *Always get sufficient sleep.*

You are strongly encouraged to communicate with instructor and with each other. Feel free to reach out to the instructor during the class, after the class, or outside of the class (via online system.)

Do all the assignments and *submit them on time*. Use this course as an opportunity to learn how to properly write up your solutions.

If you need extra challenge (or you need some catching up and some simpler exercises) – let the instructor know.

At all cost avoid getting behind and lost. Communicate your difficulties and challenges to the instructor as early as possible. To help you with this task, you will be asked to keep a *learning journal* and share it with the instructor.

## Daily Structure

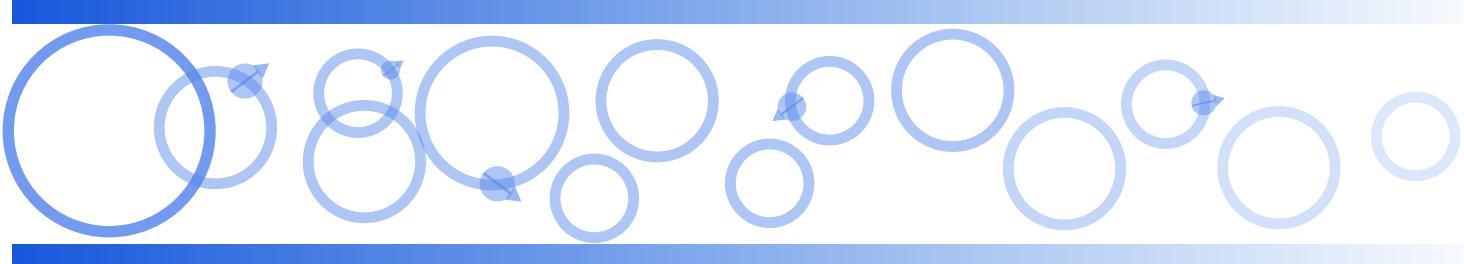
There will be four (4) classes each day: Two (2) before lunch and two (2) after.

The first “morning” class will begin with time for question from students. Instructor will accept any questions you might have. Then we will review the main points covered in the previous lecture in order to summarize and remind what we have learned.

The second “morning” class will be dedicated to learning new material and related discussions.

After lunch, the third class will also be dedicated to learning new material and related discussions.

The last class will be the time when students will work on assignments and have an opportunity to discuss topics (either with the instructor or classmates) in less formal settings. Starting from the second week of the course, students will be working on their *projects* during this time.



## Preface

*And it seems to me that at this time we need education in the obvious more than investigation of the obscure.*

---

OLIVER WENDELL HOLMES, JR.

The mechanics of Newton and Galilei is a powerfull and intuitive theory. Its successful applications to motion of planets, projectiles, pendula, bodies sliding down inclined planes, or connected via system of pullies or springs are studied by many in high school. With some effort a student can learn the language of *positions, velocities, accelerations, and forces*. For most, the education in mechanics ends there – in the framework developed by the early 18th century.

Tremendous progress in mathematics and physics, as well as other sciences, is manifested by incredible advancements of modern technologies. The language of science also evolved, it became enriched by new ideas and methods. By the mid-19 century two more views on the problems of mechanics were developed: *Lagrangian mechanics* (after Joseph Louis Lagrange), and *Hamiltonian mechanics* (after William Rowan Hamilton).

Without understanding the basics of *Lagrangian* and *Hamiltonian* mechanics, it is impossible to fully appreciate two fundamental tools: *Stationary Action Principle* and *Hamiltonian Operator* approach of quantum mechanics.

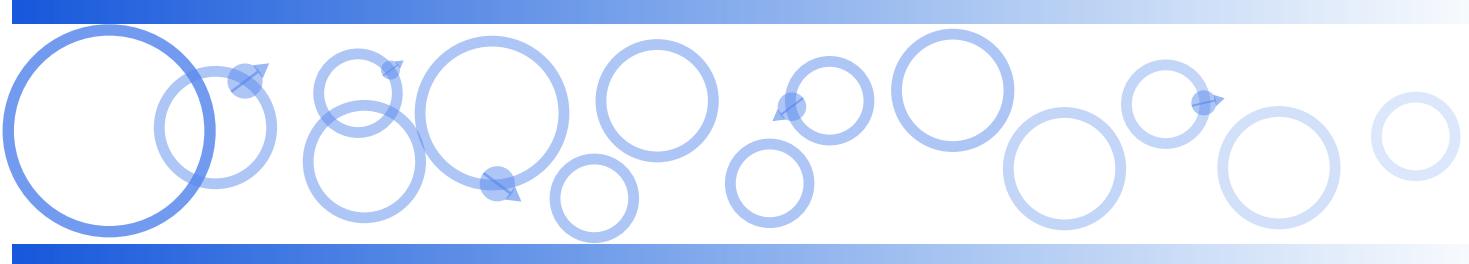
One goal of this course is to introduce students to modern language of physics. We will discuss concepts of *system, state, state evolution, equations of dynamics, Hamiltonian* and *Lagrangian* of a system, *configuration space* and *phase space*, and many more. In due time, students of physics will encounter these notions again in special courses, such as *Analytical Dynamics* and *Quantum Mechanics*. Hopefully, being introduced to the more advanced ideas and methods of physics in this course will reduce the “mental barrier” in the future encounters.

## 0.1 Quantumness

### 0.1.1 Processes, Not Properties

In the familiar picture of the world one recognizes two basic ideas: *objects* and their *properties*.

#### Key Takeaways



# 1. Introduction

Quantum physics is a notoriously difficult subject. The difficulties stem from the combination of several factors:

- Mathematical concepts and tools.
- Quantization phenomena.
- Probabilistic thinking.
- Superposition effects.
- Entanglement and non-locality.\*

Most of these factors (except the last one) are neither alien to “normal” – classical – physics, nor exceptionally difficult. Furthermore, the knowledge of classical physics helps appreciate these concepts and deepen their understanding. What sets quantum physics apart from classical physics is how these factors mesh together in a framework which is more than the sum of its parts.

## Mathematics

Mathematical tools used in quantum physics are diverse: from complex-valued functions, to calculus, to linear algebra, to group theory and more. Textbooks and papers talk about quantum states and Hilbert spaces, operators and commutators, eigen-value problems and so on. For a student of Newtonian mechanics all those appear foreign.

Take, for example, the most famous equation of quantum mechanics – Schrödinger’s equation:

$$i\hbar\partial_t|\Psi\rangle = H|\Psi\rangle. \quad (1.1)$$

Its mathematical content is made up from a special vector  $|\Psi\rangle$  and three operators<sup>1</sup>  $i$ ,  $\partial_t$ , and  $H$ . The equation states that when the operator  $\partial_t$  (rate of change with respect to time) acts on the vector  $|\Psi\rangle$ , followed by the action of the operator  $i$  (“rotation” of a vector by  $90^\circ$ ), the result will be equal to the action of the operator  $H$  on the original vector  $|\Psi\rangle$ , up to a fundamental physical constant  $\hbar$ .

<sup>1</sup>For now think of an *operator* as a kind of mathematical function that acts – operates – on its argument on the right.

From the point of view of physics, Schrödinger's equation describes how a quantum system changes its *state* with time, much like Newton's second law does in mechanics or Maxwell's equations in electrodynamics. No surprise then, that the knowledge of these classical theories is helpful. Moreover, the proficiency in Hamiltonian dynamics – a variant of classical mechanics – will definitely enhance the learning of quantum theories: the operator  $H$  in Schrödinger's equation is the quantum analog of a Hamiltonian from Hamiltonian dynamics.

These points are explained in Chapter 2.

## Quantization

When value of a physical quantity can change only in discrete steps we call such a quantity *quantized*. Quantization is the opposite of smooth, continuous change. Quantization is very natural, as suggested by the number of fingers on a hand, number of people on a bus, and so on. No surprise then, the hypotheses of granular, particulate structure of the world have a long history: from the material atoms of ancient Greek philosopher Democritus, to the light corpuscles of Isaac Newton.

Today, it is a firmly established fact that some physical quantities are quantized. The most profound discoveries of quantized quantities happened in the 20th century. First, the electromagnetic charge ( $e/3$ ), and then the unit of action ( $\hbar$ ). Several other physical quantities, related to  $e$ ,  $\hbar$  or both, are also quantized: angular momentum changes in steps of  $\hbar$ , magnetic flux – in steps of  $\Phi_0 = \hbar/2e$ , conductance of charges – in steps of  $G_0 = 2e^2/\hbar$ . (NOTE:  $\Phi_0 G_0 = e$ ).

## Probabilities

Probability is fundamental to science. All statements in physics are of probabilistic nature. We only can say that "All existing evidence makes it extremely likely, with no evidence to the contrary, that such and such law holds." Being absolutely sure is being dogmatic and that is not the spirit of science.

However, on a more technical level, the notion of probabilities came into physics with the development of the kinetic theory of gases. Starting from simple and intuitive mechanical models of atoms and molecules as colliding little balls, physicists were able to explain the law of macroscopic objects – ideal gases. Thus thermodynamics was deduced from statistical physics.

In quantum mechanics randomness and probability play different role. Randomness is not reduced to anything simpler or hidden from the superficial analysis.

## Superposition

Superposition is used in many parts of physics. The parallelogram rule for adding forces, summation of electrostatic fields from different charges, breaking motion of objects into simultaneous motion along two (or three) different

axes – these are examples of superposition used in classical physics.

In quantum physics superposition is used even to represent *states* of quantum systems. This is a major difference with some unexpected consequences, including *entanglement*.

### Brief Historical Overview

Quantum physics is an old theory. Its “official” birth-year is 1900. By 1930 the core ideas and equations have been formulated. Since then most of action has been happening in developing quantum technologies (e.g. lasers), application of quantum physics to study more and more physical systems (e.g. superconductors.), and expanding the quantum framework to all sorts of fields and interactions (quantum field theories and particle physics.)

Quantum technology has evolved through roughly three stages, as shown in the Figure 1.1. After observing quantum signatures from large groups of quantum objects (e.g. spectra of atoms and molecules), physicists were able to address single atoms, molecules, single photons. Today the challenge is to utilize subtle quantum effects involving many quantum systems.

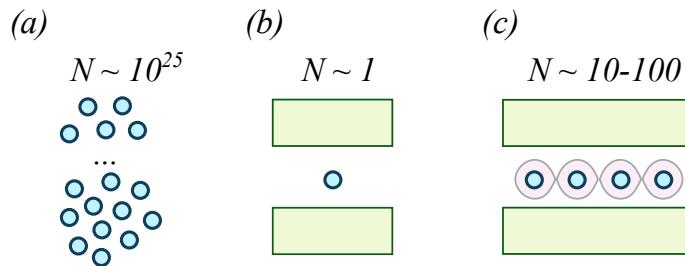


Figure 1.1: Three stages of evolution in quantum science and technology. (a) Working with large ensembles of particles (macro- and microscopic systems). (b) Working with individual atoms and single photons. (c) Working with tens and hundreds entangled quantum systems.

## Classical World

### Example

This example is due to V. Fock<sup>a</sup>. Consider a body of mass  $m$  being accelerated by some constant force. Suppose the acceleration is  $a$ . In time  $t$  the body will acquire speed  $v = at$  and kinetic energy  $K = mv^2/2$ . The action in this scenario has the magnitude on the order of

$$A = Kt \approx \frac{mv^3}{a}.$$

The accelerations we encounter in classical world are less than  $a = 100g$ . A mass is considered small if it is less than a gram  $m = 10^{-3}$  kg. A velocity of a drifting speck of dust, about millimeter per second, can be considered small:  $v = 10^{-3}$ . Plugging these numbers in, we obtain:

$$A \approx \frac{10^{-3} \times 10^{-9}}{100 \times 10} = 10^{-15} (J \cdot s).$$

Thus, even the lightest and slowest bodies in “normal” mechanics, when subjected to huge accelerations, participate in classical scenarios that involve tremendous number of action quanta:

$$A \approx 10^{19} h.$$

<sup>a</sup>On Interpretation of Quantum Mechanics, *Phys. Usp.* **4**, 1954

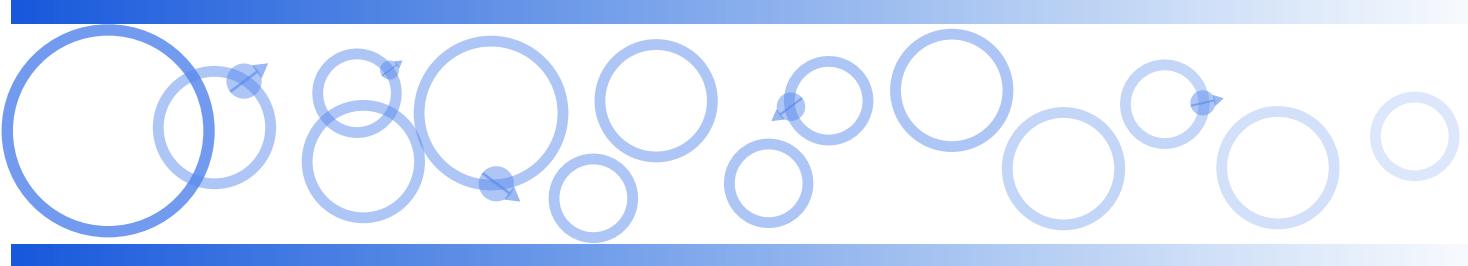
TO BE FILLED IN CLASS.

## 1.1 Quantum Paradox

Quantum physics works extremely well. Its technical part is accurate, versatile, and powerful. At the same time, numerous debates about *the meaning* of basic quantum notions, the *interpretations* of quantum physics have existed and continue to occupy many scientists.

In 1968, when quantum physics and technology has already matured, a conference of Nobel prize winners in physics has been organized in Lindau, Germany. Two of the founders, Werner Heisenberg and Paul Dirac, attended the conference. Another Nobel prize winning physicist, Willis E. Lamb, raised a simple question: “What is quantum mechanics?”

The situation can be compared to finding a powerful piece of alien technology. We seem to know how to press the buttons to get the desired result, but are unsure of what exactly those buttons mean and how they work. This is a kind of quantum paradox.



## 2. Classical Mechanics

*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.*

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P. A. M. DIRAC<sup>1</sup>

The goal of mechanics is to *describe, explain and predict* motions of mechanical systems. This is done through setting up and solving equations which describe the motion – *equations of motion*. Equations of motions describe how positions, velocities, and accelerations are connected, and how they advance through time.

The mechanics of Galileo and Newton is one possible approach the problems of motion. This approach is conceptually simple; it studies motion using velocities, accelerations, masses, and forces. Galileo-Newtonian mechanics is the first milestone in the evolution of mechanics.

About hundred years after Galileo-Newtonian mechanics, another approach was proposed by Joseph-Louis Lagrange. The mechanics of Lagrange (Lagrangian mechanics) is more abstract than Galileo-Newtonian mechanics; it introduces fundamental physical quantity: *action* and gives a guiding principle for finding equations of motions based on so called *principle of least action*. We will learn about Lagrangian mechanics in later sections.

Roughly half a century after the birth of Lagrangian mechanics, Sir William Rowan Hamilton reformulated the latter and developed a new approach to problems of motion – *Hamiltonian mechanics*. The key concept of Hamiltonian mechanics is the expression for the total energy of a system written in terms of its position and momentum; such expression is called *Hamiltonian*. Hamiltonian mechanics can be viewed as a bridge from classical to quantum physics.

The three types of mechanics – Galileo-Newtonian, Lagrangian, and Hamiltonian – address the same problem. They provide different points of view on the motions of mechanical systems. However, they share a lot of important physical concepts. We will review them next.

## 2.1 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.

A *system* is a body or several bodies interacting with each other or with some external bodies. The Figure (2.1) provides several examples of mechanical systems. Let's examine them in more detail.

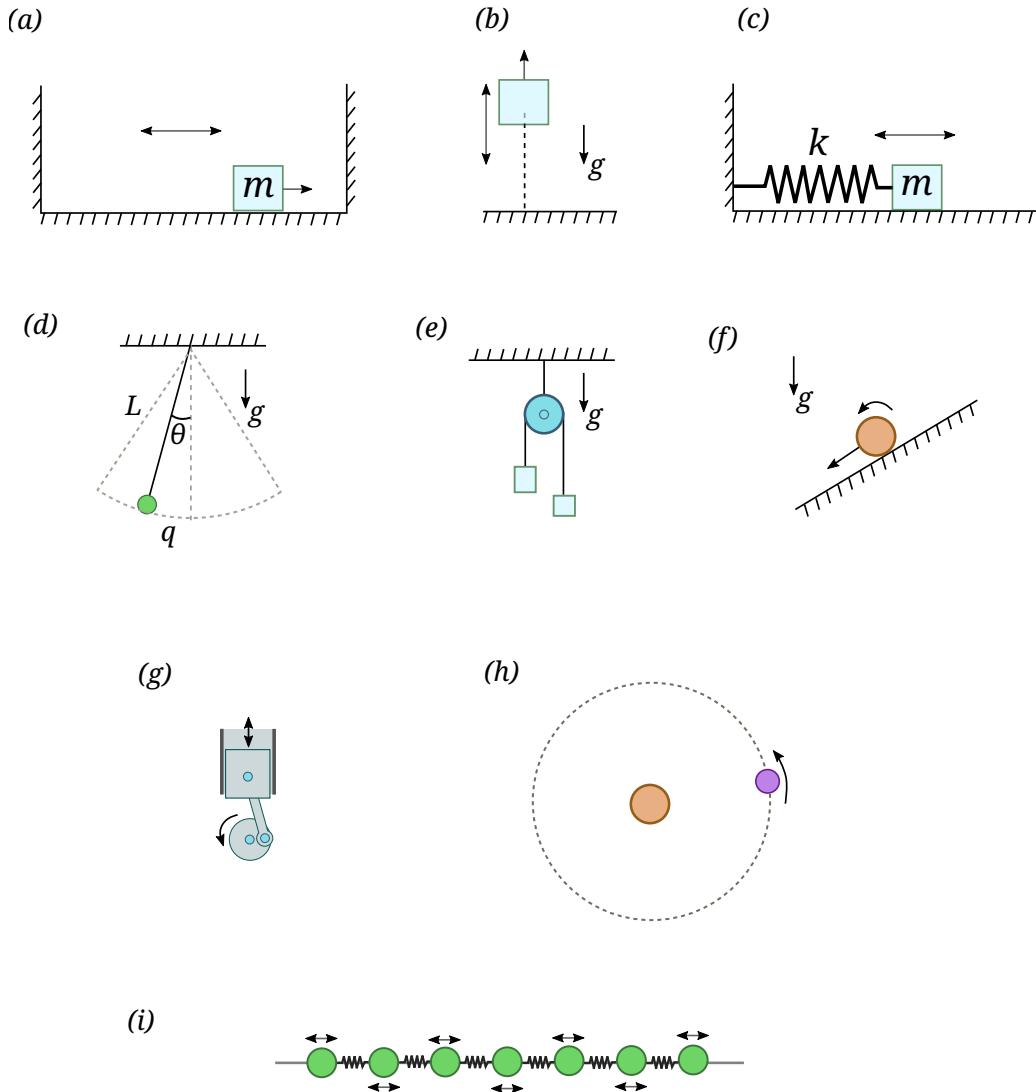


Figure 2.1: Examples of mechanical systems. See text for explanation.

- (a) *Particle in a box*: An elastic “particle” (a body) bounces between two walls, sliding across a frictionless surface.
- (b) *Free falling body*: An elastic body falls down under the force of gravity, bounces back, goes up and then down to repeat the bounce again and again.

- (c) *Spring oscillator*: A body, attached to a spring, is allowed to slide left and right across a frictionless surface.
- (d) *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.
- (e) *Atwood machine*: Two bodies with slightly unequal masses are connected with a non-stretchable string going over a frictionless pulley.
- (f) *Inclined plane*: A solid cylinder rolling down an inclined plane.
- (g) *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.
- (h) *Sun and planet*: A planet circling around the sun.
- (i) *Linear chain of oscillators*: A set of pairwise interconnected identical bodies; the allowed motion happens along the horizontal axis.

We will study the systems (a), (b), and (c) in great detail.

### 2.1.1 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 (2.2)(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 horizontal 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

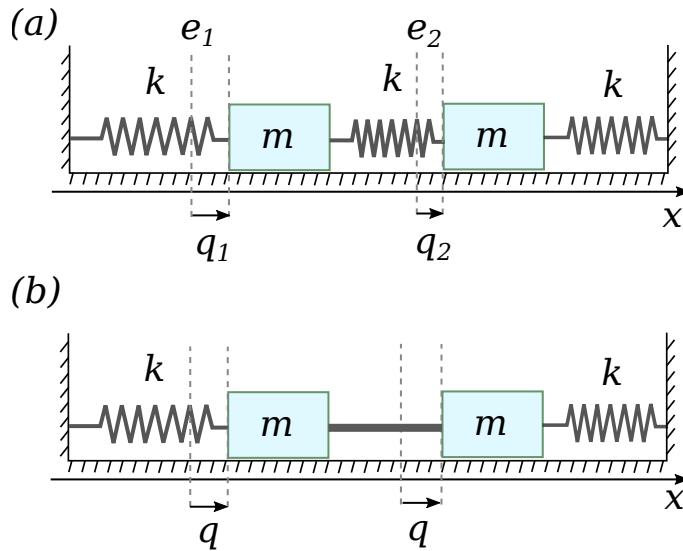


Figure 2.2: (a); (b).

this with the situation, shown in the Figure (2.2)(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.

### 2.1.2 Generalized Coordinates

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 (2.1)(b).

Consider another example, shown in the Figure (2.1)(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.

### 2.1.3 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 (2.3). 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.

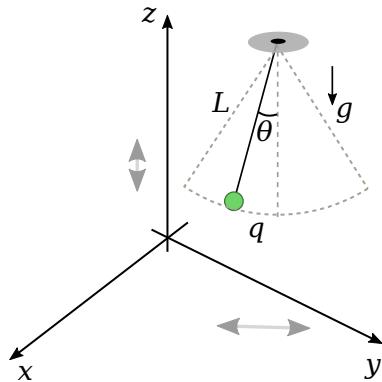


Figure 2.3: A pendulum has one degree of freedom, despite the fact that all three Cartesian coordinates can be changing during its motion.

## 2.2 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.

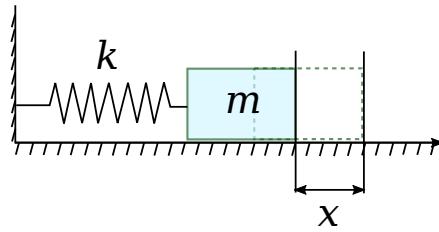


Figure 2.4: A mechanical model of an oscillator: A body attached to an ideal spring.

Consider a body with the mass  $m$  is attached to a spring with the stiffness  $k$ . The body is allowed to move across an ideally smooth (no friction) surface. 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 body, 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

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

Finally, the force required to stretch 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 opposite direction.

### 2.3 State

*State* of a system is the 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 the 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  $\delta t$ . The first iteration results in the updated value of position

$$x_1 = x_0 + v_0 \delta t. \tag{2.1}$$

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

$$x_2 = x_1 + v \delta t \tag{2.2}$$

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 the acceleration:

$$v_1 = v_0 + a_0 \delta t. \quad (2.3)$$

Once this is done, 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:

$$a_1 = a_0 + b_0 \delta t, \quad (2.4)$$

but this is not required. At this point we can use the laws of motion. For example, the Newton's second law allows us to find the acceleration, if we know the force acting on the object:

$$a = \frac{F}{m}. \quad (2.5)$$

All physical forces, it appears, depend on positions (distances) and, sometimes, velocities of bodies. The force of the spring, for example, depends only on the coordinate  $x$ . The force of gravitational interaction and the Coulomb force between two charges both depend on the distance  $r$  between the bodies. The force acting on an electron moving through a magnetic field depends on the electron's velocity. 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:

$$a_n = \frac{F(x_n, v_n)}{m}. \quad (2.6)$$

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 position, 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.

### 2.3.1 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 make a single tick after a tiny time interval  $\delta t$  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  $(x_0, v_0)$  to  $(x_1, v_1)$ . At this point we can keep repeat 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 and write a mathematical function

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

Using this simple approach, we can calculate the state  $(x, v)$  of the oscillator for any moment in the future or past. The Figure 2.5 shows two example results. The first result, in the column (a), demonstrates that we must be careful with the step size  $\delta t$  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

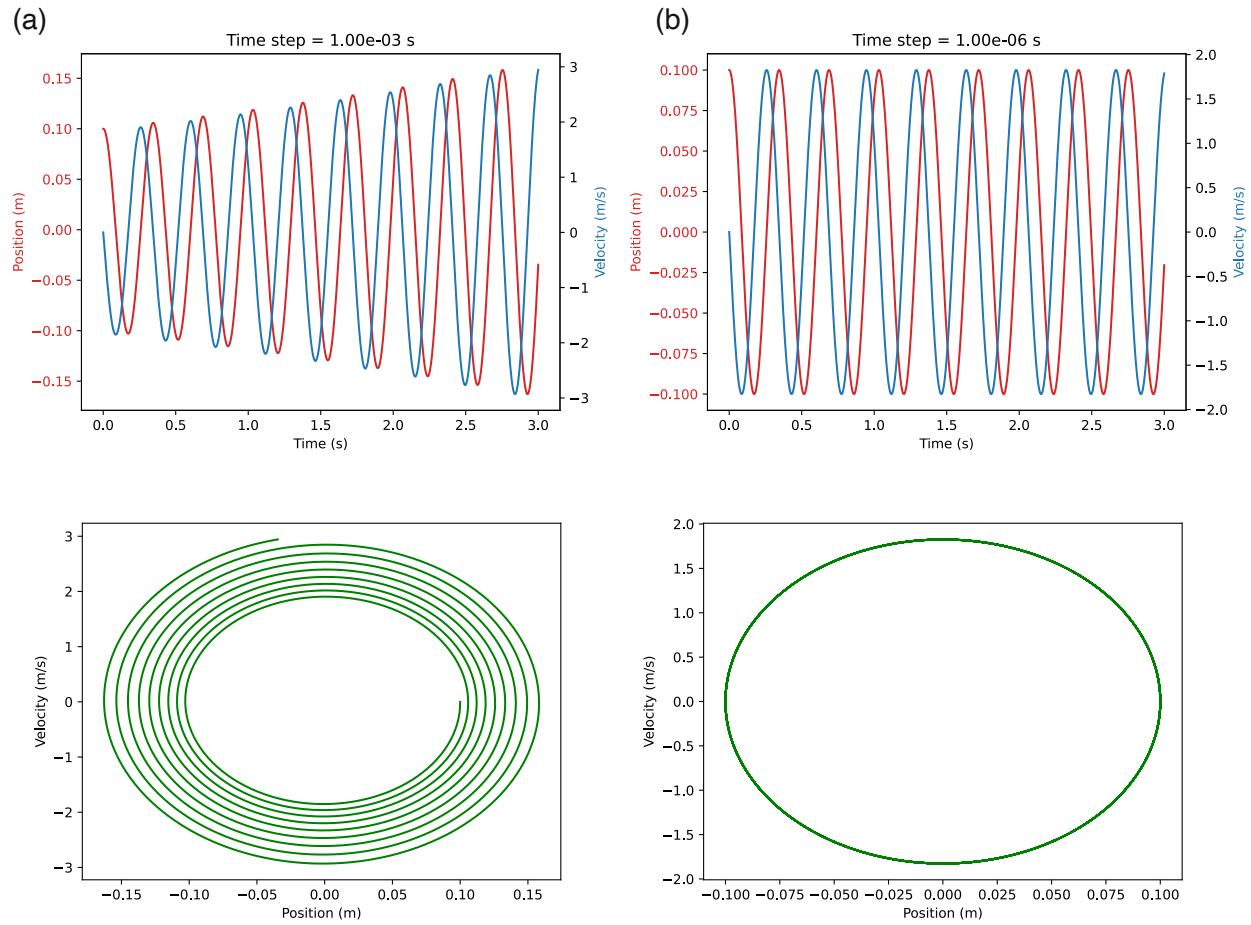


Figure 2.5: First row: Position (red curve, left axis) and velocity (blue curve, right axis) as functions of time. Second row: Velocity vs position. (a) Calculations with time step of 1 millisecond. (b) Calculations with time step of 1 microsecond.

column (b) of the Figure 2.5 demonstrates the expected behavior of the oscillator – periodic change of position with constant amplitude.

## 2.4 Hamiltonian

*Hamiltonian* is the expression for the total energy of a system, written in terms of *position* and *momentum*.

### Schrödinger on Hamiltonian

The central conception of all modern theory is “the Hamiltonian.” If you wish to apply modern theory to any particular problem, you must start with putting the problem “in Hamiltonian form.”

Thus Hamilton is one of the greatest men of science the world has produced.

“*The Hamilton Postage Stamp: an Announcement by the Irish Minister of Posts and Telegraphs*,” in “*A Collection of Papers in Memory of Sir William Rowan Hamilton*,” ed. David Eugene Smith, Scripta Mathematica Studies, no. 2 (New York: Scripta Mathematica, 1945), 82

We will limit ourselves to motions with speeds much smaller than the speed of light. For such motions, the expression for momentum is

$$p = mv.$$

### Problem

Write down the Hamiltonians of our three main systems: (a), (b), and (c) in the Figure (2.1).

## 2.5 Dynamics

The total energy of an oscillator is the sum of its kinetic and potential energies:

$$E = E_k + E_p = \frac{mv^2}{2} + \frac{kx^2}{2}. \quad (2.7)$$

To rewrite it in terms of momentum, recall that the momentum, in classical physics, is the product of mass and velocity –  $p = mv$ . Plugging this into the expressio for the energy we obtain

$$H = \frac{p^2}{2m} + \frac{kx^2}{2}, \quad (2.8)$$

here we denoted the energy with the letter  $H$  – for Hamiltonian.

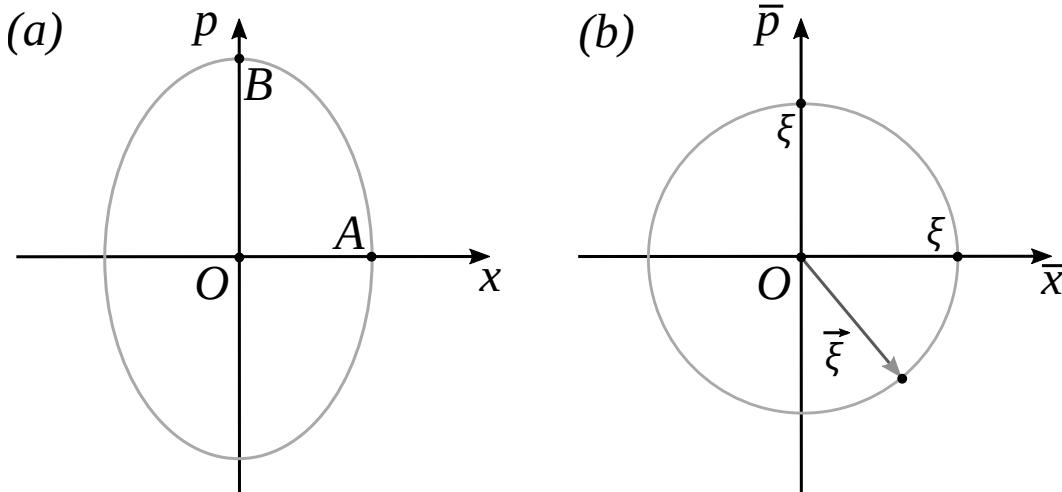


Figure 2.6: (a) During the motion, both the position  $x$  and momentum  $p$  change, while the point  $P = (x, p)$  remains on the ellipsis. (b) The motion of the oscillator in the normalized coordinates  $\bar{x}$  and  $\bar{p}$  is described by a circle with the radius  $\xi = \sqrt{\bar{H}}$ . A particular combination of  $\bar{x}$  and  $\bar{p}$  can be described by a state vector  $\vec{\xi} = \bar{x} + \bar{p}\hat{J}$ .

While both  $x$  and  $p$  change during the motion of the oscillator, their combination satisfies the relation:

$$1 = \frac{x^2}{2H/k} + \frac{p^2}{2mH}, \quad \text{compare to} \quad 1 = \frac{x^2}{a^2} + \frac{y^2}{b^2}.$$

Thus, in the  $xp$  plane this equation describes an ellipsis, as illustrated in the Figure 2.6(a).

The analysis of the oscillator motion can be simplified if we make the equation (2.8) dimensionless: instead of the usual units for distance ( $m$ ), momentum ( $kg * m/s$ ), and energy ( $J$ ), we will express them as scaled versions of some “natural” values  $x_0$ ,  $p_0$ , and  $H_0$ :

$$x = \bar{x}x_0, \quad p = \bar{p}p_0, \quad H = \bar{H}H_0,$$

where  $\bar{x}$ ,  $\bar{p}$ ,  $\bar{H}$  are unitless quantities.

For the body with mass  $m$ , we will use as the “natural energy” value the rest-energy of an electron:

$$H_0 = m_e c^2.$$

An oscillator with such energy will have the maximum displacement:

$$x_0 = \sqrt{\frac{2H_0}{k}}, \quad \text{and maximum momentum} \quad p_0 = \sqrt{2mH_0}.$$

Now the Hamiltonian can be written in dimensionless units:

$$\bar{H}H_0 = \frac{kx_0^2}{2}\bar{x}^2 + \frac{p_0^2}{2m}\bar{p}^2 = H_0\bar{x}^2 + H_0\bar{p}^2.$$

The relationship between the position and momentum is therefore described by the equation of a circle in  $\bar{x}\bar{p}$

plane:

$$\bar{H} = \bar{x}^2 + \bar{p}^2.$$

The state of the oscillator is therefore specified by a point in the  $\bar{x}\bar{p}$  plane and can be described by a compound number (a state vector):

$$\hat{\xi} = \bar{x}\hat{I} + \bar{p}\hat{J} = \bar{x} + \bar{p}\hat{J};$$

see the Figure 2.6(b). It is customary to drop  $\hat{I}$  from the expression involving operators, as long as it is clear from the context that it must be there.

Hamiltonian has two very important properties. First, it is a *conserved quantity* – the total energy is conserved if there are no external forces (e.g. friction). Second, and this is very important, Hamiltonian contains in itself information about the laws of motion. To see this, consider the oscillator at two close moments of time:  $t$  and  $t + \delta t$ . Although both the position and velocity (and momentum) will change, their combination which comes into the expression for the energy, remains constant. Let's denote the position, the velocity, and the momentum of the oscillator at the moment of time  $t + \delta t$  as follows:

$$x + \delta x, \quad v + \delta v, \quad p + \delta p.$$

The Hamiltonian will have the same numerical value

$$H = \frac{(p + \delta p)^2}{2m} + \frac{k(x + \delta x)^2}{2}. \quad (2.9)$$

Subtracting the expression of the Hamiltonian at the time  $t$  from this equation, results in

$$0 = \frac{(p + \delta p)^2 - p^2}{2m} + k \frac{(x + \delta x)^2 - x^2}{2}. \quad (2.10)$$

To simplify, we use the algebraic identity  $a^2 - b^2 = (a - b)(a + b)$ , to get

$$\frac{(2p + \delta p)\delta p}{2m} + \frac{k(2x + \delta x)\delta x}{2} = 0. \quad (2.11)$$

Next, using the facts that  $\delta x = v\delta t$ , and  $\delta p = m\delta v = ma\delta t$ , we rewrite the last expression

$$\frac{(2p + ma\delta t)ma\delta t}{2m} + \frac{k(2x + v\delta t)v\delta t}{2} = 0. \quad (2.12)$$

Diving everything by  $\delta t/2$ , and canceling the mass  $m$  in the first term, we arrive at

$$(2p + ma\delta t)a + k(2x + v\delta t)v = 0. \quad (2.13)$$

Now, we consider the motion of a system in very small steps, where  $\delta t$  is has a tiny value. Mathematicians use the approach where they consider what happens in the limit when  $\delta t \rightarrow 0$ , whereas applied physicists content with the fact that any term with  $\delta t$  is vanishingly small and can be neglected; such terms can be made arbitrarily small, by making the time step  $\delta t$  as small as required. With this in mind, we write the previous expression as follows:

$$2pa + 2kxv = 0. \quad (2.14)$$

The last step is to use the fact that  $p = mv$ , and, after cancelation of the factor  $2v$ , write

$$ma = -kx = F_{spring}. \quad (2.15)$$

This the law of motion, identical to the one given by the Newton's second law. Thus, the conservation of energy, combined with the relationships between the momentum and velocity, kinetic energy and momentum, potential energy and position, lead to the same equation of motion as using Newton's law of dynamics. Although it seems like we gained a little in this exercise, and had to follow a longer route to the same equation, the use of Hamiltonian is a powerful technique, which extends into the problems that do not afford the notion of a force.

### 2.5.1 Hamiltonian Equations

In the Newtonian mechanics, the state of a mechanical system is given by a pair  $(x, v)$ . In Hamiltonian dynamics, the state is given the pair  $(x, p)$ , for which we will introduce a special notation, using a single Greek letter  $\xi$ :

$$|\xi\rangle = (x, p) = x + \hat{J}p. \quad (2.16)$$

We now find the equations that allow to advance the values of  $x$  and  $p$  in time, and thus predict the state at a moment of time  $t$ , starting from the value of the state at some initial moment of time  $t_0$ . The important result, however, will be not just the equations themselves, but their connection to the Hamiltonian, as we want to stay completely within the framework of Hamiltonian dynamics. We will continue using the oscillator model, described above.

The change of position  $\delta x$  is determined by velocity. The latter is connected to the momennum:  $v = p/m$ .

Figure 2.7: Schematic representation of Hamiltonian as function of position and momentum.



Therefore,

$$\delta x = \frac{p}{m} \delta t \quad (2.17)$$

The change of momentum  $\delta p$  is determined by the force, as the Newton's second law states.

$$\delta p = F \delta t = -kx \delta t. \quad (2.18)$$

The right-hand sides of the equations for  $\delta x$  and  $\delta p$  do not explicitly depend on the Hamiltonian. Now we will find how to fix this. We start with the expression for the Hamiltonian of the oscillator

$$H = \frac{p^2}{2m} + \frac{kx^2}{2}. \quad (2.19)$$

Viewed from a purely mathematical standpoint,  $H$  is a function two variables –  $x$  and  $p$  (to be precise, it is a function of four variables –  $x$ ,  $p$ ,  $m$ , and  $k$ .) This function works like a box with two inputs and one output, as shown in the Figure below.

Changing  $x$  results in the change of the value of the Hamiltonian. Similarly, changing  $p$  leads to the change of the Hamiltonian value. The unique feature of the actual motion of the oscillator (and other mechanical systems) is that, firstly, both position and momentum change during the motion. Secondly, and more importantly, the change  $\delta x$  and  $\delta p$  are related *in a very specific way*, which ensures that the value for the Hamiltonian remains constant, despite the change of the inputs.

Consider a slight change of the position only. The Hamiltonian will change and becomes

$$H + \delta H = \frac{p^2}{2m} + \frac{k(x + \delta x)^2}{2} \quad (2.20)$$

Subtracting the initial value for the Hamiltonian, we find

$$\delta H = \frac{k[(x + \delta x)^2 - x^2]}{2} = \frac{k(2x + \delta x)\delta x}{2} \quad (2.21)$$

Dividing both sides by  $\delta x$  and taking into account that  $\delta x \ll 2x$  (or taking the limit of  $\delta x \rightarrow 0$ ), we arrive at

$$\frac{\delta H}{\delta x} = kx \quad (2.22)$$

Next, consider a slight change of momentum only. The Hamiltonian will change to

$$H + \delta H = \frac{(p + \delta p)^2}{2m} + \frac{kx^2}{2}. \quad (2.23)$$

Subtracting the initial value  $H$  of the Hamiltonian results in

$$\delta H = \frac{[(p + \delta p)^2 - p^2]}{2m} = \frac{(2p + \delta p)\delta p}{2m}. \quad (2.24)$$

Dividing both sides of the equality by  $\delta p$ , and taking into account that  $\delta p$  is vanishingly small, we get

$$\frac{\delta H}{\delta p} = \frac{p}{m}. \quad (2.25)$$

Now we are ready to connect the changes in  $x$  and  $p$  to the Hamiltonian. Firstly, note that

$$\delta x = \frac{p}{m}\delta t = \frac{\delta H}{\delta p}\delta t, \quad (2.26)$$

and, secondly,

$$\delta p = -kx\delta t = -\frac{\delta H}{\delta x}\delta t. \quad (2.27)$$

Using  $\partial$ -notation, we can make equations look more neat and compact. First,

$$\frac{\delta x}{\delta t} = \frac{\delta H}{\delta p} \quad \rightarrow \quad \partial_t x = \partial_p H, \quad (2.28)$$

and then

$$\frac{\delta p}{\delta t} = -\frac{\delta H}{\delta x} \quad \rightarrow \quad \partial_t p = -\partial_x H \quad (2.29)$$

These are *Hamiltonian Equations of Motion*. They express how the state  $|\xi\rangle = (x, p)$  of a mechanical system changes in time, by relating the rates of change of  $x$  and  $p$  to the Hamiltonian.

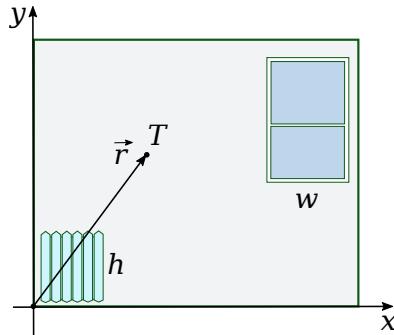


Figure 2.8: Air temperature in the room with a heater and a window changes from point to point.

### Single Hamiltonian Equation

There are two equations in Hamiltonian dynamics: one for position  $x$ , the other for momentum  $p$ . In applications, when numerically calculating these quantities, two equations are used separately. However, when studying the motion of various mechanical systems mathematically and generally, it is convenient to combine two equations into one.

The situation is analogous to the use of vectors in Newtonian mechanics. For example, for a general motion in three dimensions, the Newton's second law is written as

$$\vec{F} = m \vec{a}, \quad (2.30)$$

which is a compact form of three equations, one for each coordinate axis

$$F_x = ma_x, \quad F_y = ma_y, \quad F_z = ma_z.$$

A vector notation  $\vec{a} = (a_x, a_y, a_z)$  is used to greatly improve the economy of mathematical manipulations.

We can write compactly

$$\delta|\xi\rangle = (\delta x, \delta p) \quad \text{and} \quad \partial_t|\xi\rangle = (\partial_t x, \partial_t p). \quad (2.31)$$

Another notational tool is often used in connection to the “rate of change”. Consider a situation, shown in the Figure below.

The temperature  $T$  in a room with a heater and a window will be different in different locations. Mathematically,  $T$  is a function of coordinates  $x$  and  $y$ :  $T(x, y)$ . A point inside the room can also be specified by an arrow (a vector)  $\vec{r}$ , and the temperature can be viewed as the function of such a vector:  $T(\vec{r})$ . The “sensitivity” of  $T$  to the coordinate  $x$ , or the rate of change of  $T$  with respect to  $x$ , is given by

$$\frac{\delta T}{\delta x} = \partial_x T. \quad (2.32)$$

Similar expression can be written for the coordinate  $y$ :

$$\frac{\delta T}{\delta y} = \partial_y T. \quad (2.33)$$

These two quantities can be combined similar to the components of a vector, and written as a single expression

$$\frac{\delta T}{\delta \vec{r}} = \partial_{\vec{r}} T = (\partial_x T, \partial_y T) \quad (2.34)$$

Using this approach, the “sensitivity” of the Hamiltonian to position  $x$  and  $p$  can be written as a single expression – the sensitivity of the Hamiltonian to a state:

$$\frac{\delta H}{\delta \xi} = \partial_{\xi} H = (\partial_x H, \partial_p H). \quad (2.35)$$

The rate of change of a state  $|\xi\rangle$  with respect to time is determined by the Hamiltonian of the system, as we demonstrated:

$$\partial_t |\xi\rangle = (\partial_t x, \partial_t p) = (\partial_p H, -\partial_x H). \quad (2.36)$$

The right-hand side of this equation depends on the Hamiltonian and looks somehow related to the rate of change of the Hamiltonian with respect to the state  $\partial_{\xi} H$ . To establish the proper relationships we can use *compound numbers*.

### Compound Numbers in Hamiltonian Dynamics

First note that

$$\partial_t |\xi\rangle = \partial_p H - J \partial_x H \quad (2.37)$$

Applying an operation  $J$  to both sides (“multiplying” by  $J$  both sides), results in

$$J \partial_t |\xi\rangle = J \partial_p H - J \cdot J \partial_x H = \partial_x H + J \partial_p H \quad (2.38)$$

Comparing this with the expression for the rate of change of the Hamiltonian with respect to the change of state

$$\partial_{\xi} H = (\partial_x H, \partial_p H) = \partial_x H + J \partial_p H \quad (2.39)$$

we can conclude that

$$J\partial_t|\xi\rangle = \partial_\xi H. \quad (2.40)$$

This is a single formula, combining two equations of Hamiltonian dynamics. Its main message is that Hamiltonian of a mechanical system completely determines how the state  $|\xi\rangle = (x, p)$  changes in time.

To arrive at a short expression for the evolution of a state, we had to use several mathematical abstractions, including the idea of a rotation operation  $J = \sqrt{-1}$ . We are now able to compare the compact version of the Hamiltonian equations to the Schrodinger's equation:

$$i\partial_t\Psi = \frac{1}{\hbar}H\Psi. \quad (2.41)$$

The meaning of the terms involved into this equation is the following:  $\Psi$  is the state of a quantum system (*quantum state*);  $i$  is the complex number ( $i^2 = -1, i = \sqrt{-1}$ ), with the same meaning as the operation  $J$ ;  $H$  is the Hamiltonian of a quantum system;  $\partial_t$  is the way to find the rate of change of any quantity with respect to time. Schrodinger's equations expresses how the evolution of a quantum state is determined by the Hamiltonian of a quantum system; similar to how the classical Hamiltonian determines the evolution of a state of a classical mechanical system. Schrodinger equation can be “decomposed” into two separate equations, since the quantum state  $\Psi$  has two parts (components):

$$\Psi = \Psi_1 + i\Psi_2, \quad (2.42)$$

- a situation analogous to the classical state  $|\xi\rangle = x + Jp$ .

Lastly, the presence of the quantity  $\hbar$  in Schrodinger's equation can be understood after we learn more about the quantization features of quantum physics.

### Hamiltonian Framework

Hamiltonian approach is not limited to mechanics. Equations similar to Hamiltonian equations can be written for electromagnetic field without charges. They can look as follows:

$$J\partial_t\psi = A\psi.$$

Here  $\psi = E + JH$ , where  $E$  is electric field,  $H$  is magnetic field, and  $A$  is a linear operator involving operators  $\partial_x$  and  $\partial_t$ .

The equations for gravitational field also can be put into Hamiltonian form, as was shown by R. Arnowitt, S. Deser, and C. W. Misner. In their approach – called the ADM formalism – the gravitational potential  $g$  and its momentum  $\pi$  change with time according to the equations

$$\begin{aligned}\partial_t g &= F_1(g, \pi), \\ \partial_t \pi &= F_2(g, \pi).\end{aligned}$$

Hamiltonian framework encodes simple, but important, idea of *deterministic* evolution of a state: From the knowledge of a system at some moment  $t$ , one can find all required knowledge about the system at a later moment  $t + \delta t$  (or an earlier moment  $t - \delta t$ ).

For oscillator the evolution of the state vector  $|\xi\rangle$  in time is described by a simple equation. We will “derive” it now.

As the time advances by a small amount  $\delta t$ , the state vector also changes by a small amount:

$$\delta|\xi\rangle = \delta\bar{x} + \delta\bar{p}\hat{J}.$$

On the other hand, since the tip of the state vector follows along the circle of radius  $\xi = \sqrt{H}$ , its change can be written as

$$\delta|\xi\rangle = -\delta\phi\xi \times \hat{J}\left(\frac{|\xi\rangle}{\xi}\right) = -\delta\phi\hat{J}|\xi\rangle.$$

If we denote the rate of change of the angle  $\phi$  as  $\omega = \frac{\delta\phi}{\delta t}$ , we will arrive the equation for the state evolution:

$$\frac{\delta|\xi\rangle}{\delta t} = -\omega\hat{J}|\xi\rangle. \quad (2.43)$$

### Hamiltonian Equations

The left-hand side of (2.43) can be written in terms of the position and momentum:

$$\frac{\delta|\xi\rangle}{\delta t} = \frac{\delta\bar{x}}{\delta t} + \frac{\delta\bar{p}}{\delta t}\hat{J}.$$

Doing the same with the right-hand side of the equation (2.43), we obtain

$$-\omega\hat{J}|\xi\rangle = p\omega - \omega x\hat{J}.$$

We thus derived the time-evolution equations for position and momentum:

$$\frac{\delta\bar{x}}{\delta t} = \omega\bar{p}, \quad \frac{\delta\bar{p}}{\delta t} = -\omega\bar{x}.$$

These equations represent *Hamiltonian equations* for oscillator. The equations are central to *Hamiltonian dynamics*. Hamiltonian dynamics is an approach to mechanics alternative to Newtonian dynamics. Instead of using the concept of forces and Newton's second law, Hamiltonian dynamics uses the concept of Hamiltonian.

For the oscillator, the angular speed  $\omega$  turns out to be constant. To show this, first notice

$$\frac{\delta\bar{x}}{\delta t} = \frac{\delta x}{x_0\delta t} = \frac{v}{x_0} = \frac{p}{mx_0} = \frac{p_0}{mx_0}\bar{p}.$$

Then compare this to the first equation of motion to find

$$\omega = \frac{p_0}{mx_0} = \sqrt{\frac{k}{m}},$$

where the last result is obtain by substituting the expressions for  $x_0$  and  $p_0$  in terms of the energy  $H_0$ .

Another illuminating relationship exists between the angular speed  $\omega$  and the energy  $H_0$ . To find it we can use the fact

$$\frac{p_0}{m} = \frac{2H_0}{p_0} \quad \text{and arrive at} \quad \omega = \frac{2H_0}{x_0p_0}.$$

This expression allows us to write the time-evolution equation for the state vector  $|\xi\rangle$  in *Schrödinger form*:

$$\hat{J}h_0\frac{\delta|\xi\rangle}{\delta t} = H_0|\xi\rangle, \tag{2.44}$$

where  $h_0 = x_0 p_0$  is the quantity with the units of angular momentum, or energy multiplied by time. Such quantity is known as *action*. Compare this equation to the *Schrödinger equation*:

$$i\hbar \frac{\delta |\Psi\rangle}{\delta t} = \hat{H}|\Psi\rangle.$$

Having shown that the angular speed  $\omega$  is constant, we deduce the time dependence of position and momentum for the oscillator:

$$x = x_0 \xi \cos \omega t.$$

Given that

$$\xi = \sqrt{\frac{H}{H_0}} = \frac{A}{x_0} = \frac{B}{p_0},$$

where  $A$  is the maximum displacement of the oscillator with the energy  $H$ , we can write

$$x = A \cos \omega t, \quad p = B \sin \omega t,$$

where

$$A = \sqrt{\frac{2H}{k}}, \quad B = \sqrt{2Hm}.$$

This is the mathematical description of the *oscillatory motion*.

## 2.6 Lagrangian

Mechanical system can be characterized by its total energy  $E(x, v)$  or  $H(q, p)$ . It can also be characterized by a kind of “energy imbalance” which is more formally called *Lagrange function* or *Lagrangian* of a system.

For a mechanical system with kinetic energy  $E_k(q, v)$  and potential energy  $E_p(q)$ , Lagrange function can be calculated as follows:

$$L = E_k - E_p.$$

The units for Lagrange function are the same as the units for energy or Hamiltonian (Joules in International System SI), but the meaning and use of Lagrange function is what sets it apart from other functions of the state of a mechanical system.

### 2.6.1 Stationary Action Principle

Although mathematically Lagrange function 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 important 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  $q(t)$ . This function immediately determines the velocity  $v(t) = \partial_t q$ . 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:

$$A = \int L(t)\delta t.$$

#### 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 motion  $q(t)$  physically allowable 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  $q_*(t)$  for which the value of action  $A$  is *stationary* or *extreme* – either maximal or minimal and insensitive to small deviation of the motion  $q(t)$  from its “true” form  $q_*(t)$ . This is the essence 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:

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

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

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

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:

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

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.

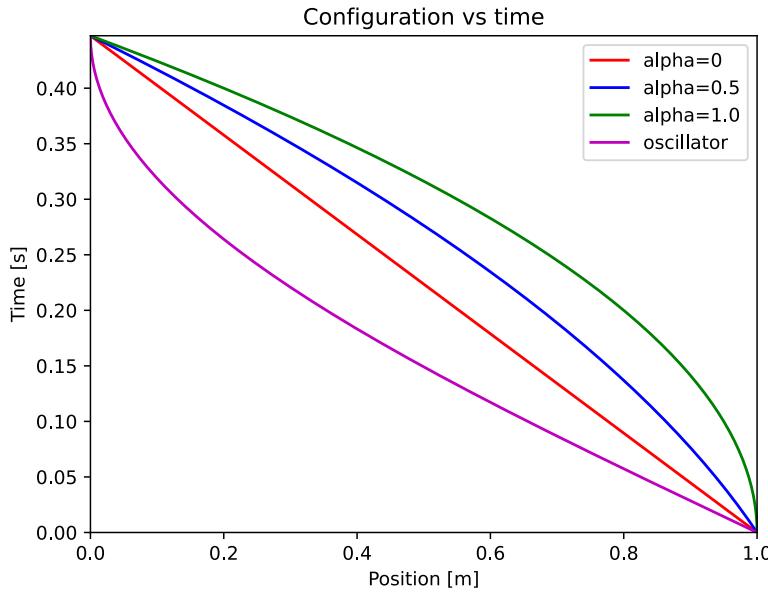


Figure 2.9: Different types of vertical motion in Lagrange picture. Particles start and stop at the same times and in the same places, moving between initial and final configurations according to different equation  $q(t)$ .

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:

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

Plugging in the expressions for velocity, we arrive at

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

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

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

Examining the expression for the total action, we see that  $A$  depends on the “mixing” parameter  $\alpha$  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:

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

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

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

The coefficient in front of  $\alpha^2$  is

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

Finally, the total action depends in the parameter  $\alpha$  as

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

To find the condition for extremal/stationary action, we need to find  $\alpha$  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 2.1** 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  $\alpha$  for which the action  $A(\alpha)$  becomes stationary. ■

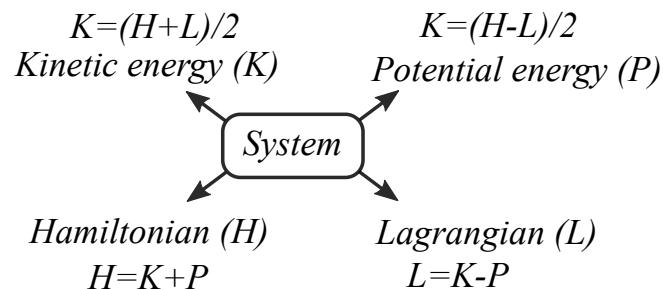
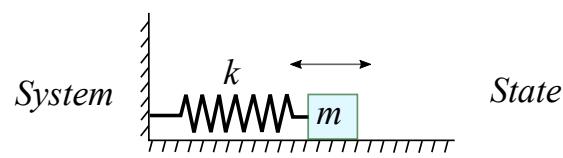


Figure 2.10: System can be described either by kinetic and potential energies, or Hamiltonian, or Lagrangian.

## 2.7 Limitation of Classical Physics

According to classical physics atoms can not exist. That should be enough. Also, a point-like electron produces electric field that has infinite total energy.

TO BE FILLED IN CLASS.

## 2.8 Ideal Vs Real Mechanics

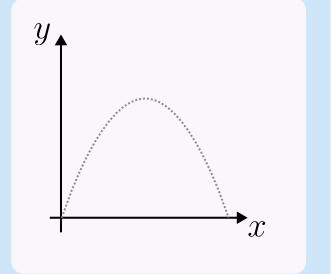
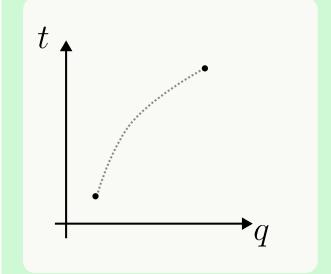
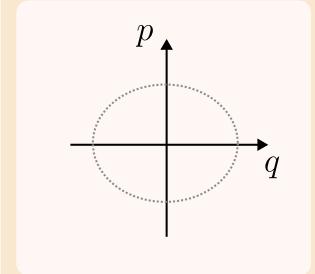
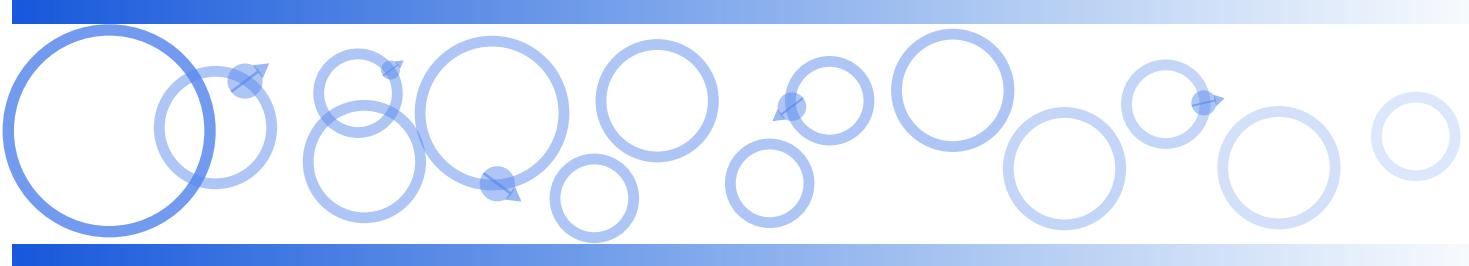
| Dynamics             |   |  |   |
|----------------------|---|--|---|
|                      | Newtonian<br>1687   | Lagrangian<br>1788   | Hamiltonian<br>1833   |
| <b>Description</b>   | $x(t), y(t), z(t)$  | $q_1(t), q_2(t), \dots, q_n(t)$  | $q(t), p(t)$  |
| <b>State</b>         | $\xi = (x, v)$  | $\xi = (q, \dot{q})$   | $\xi = (q, p)$  |
| <b>Equation</b>      | $m\vec{a} = \vec{F}$  | $p = \partial_{\dot{q}}L \quad \dot{p} = \partial_q L$                               | $J\partial_t\xi = \partial_\xi H$   |
| <b>Driver</b>        | $\vec{F}$   | $L = K - \Pi$  | $H = K + \Pi$   |
| <b>Visualization</b> |  |  |  |
|                      | <b>Trajectory</b>   | <b>Path</b>  | <b>Trajectory</b>   |

Figure 2.11: Summary of three different approaches to problems of motion.



## 3. Quantum Mechanics

Quantum physics makes heavy use of vectors and operators, as well as of compound numbers (or complex numbers). These mathematical tools are not exclusive to quantum physics. Classical physics uses similar mathematical tools; it also shares many fundamental physical concepts with quantum physics, such as *system*, *state*, *state evolution*, *dynamical equation*, and many more.

### 3.1 Quantum System

*Quantum system* is any physical object, or a group of objects, exhibiting behavior inconsistent with classical physics. Examples are:

- Electron
- Atom
- Atomic nucleus
- Molecule
- Weak light (low-intensity light)

Common to all these examples is their sub-microscopic size and small number of “particles”. This might give a *false impression* that quantum physics only applies at atomic or molecular scale. Quantum physics is also essential for understanding many *macroscopic* phenomena, involving many “bodies”; examples are the behavior of metals and semiconductors, especially at low temperatures. Several examples of quantum systems are schematically shown in the Figure 3.1.

Parameters determining whether the behavior of a system is classical or quantum are *action* and *coherence*. Essentially, if processes in a physical system involve action on the order of quantum of action  $A_0 = h$ , the system should be considered using quantum theory. Similarly, when the *phase* information of the system remains stable, then quantum theory is needed to treat the behavior of the system under study.

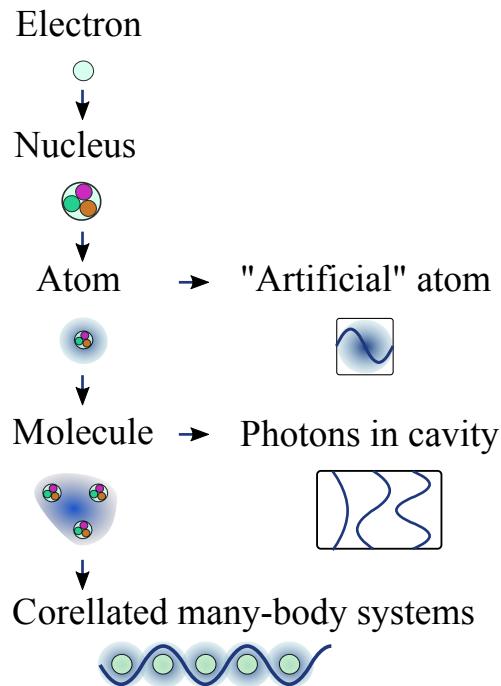


Figure 3.1: Several examples of typical quantum systems.

### 3.2 Quantum State

Classical notion of a state, based on generalized positions and momenta, has a quantum sibling – *quantum state*, which is simply the state of a quantum system. Quantum state must contain all information about the quantum system, sufficient to calculate the state of the system in the future, given its state now. Physically and mathematically, quantum state differs significantly from the classical state, as we will soon learn.

In quantum physics, the idea of a state is as important as in classical physics. However, careful analysis of the measurements of position  $x$  and momentum  $p$ , reveals that these two observables are intimately connected and *can not be known precisely at the same time*. In the process of locating an electron, for example, any measurement apparatus will have to interact with the latter, and thus affect the electron's momentum. Analogously, a precise measurement of momentum will result in large uncertainty in the location of a particle.

The classical idea of a state as a pair of position and momentum  $(x, p)$  does not work in quantum physics. Instead, a *quantum state* is used:

$$\vec{\xi} \rightarrow |\Psi\rangle,$$

where different notation is used for quantum state, proposed by Paul Dirac and known as *Dirac notation*. The concept of the state remains the same: State is all the physical information there is to know about a system. Given

the state now, we can compute the state at any other moment.

### 3.2.1 State Representation

Mathematical description of a quantum state is similar to the description of a vector. Important property of a vector is that it is not reduced to its components; the components of the same vector are different in different coordinate systems. The components of a vector merely *represent* the vector in specific coordinates.

Quantum states are vectors: They can be added, multiplied, their lengths can be calculated, and they can be *represented* via components in specific “coordinate system”. Two most important representations of quantum states are *coordinate representation* and *momentum representation*.

### 3.2.2 State Notation

Notation is a tool of thought. Clear and powerful notation makes reasoning and mathematical manipulations easy and transparent, saving time and effort. Modern notation in quantum mechanics was introduced by Paul Dirac in 1939.<sup>1</sup> Dirac’s notation is convenient and widely used.

In Dirac’s notation quantum state is denoted by an arbitrary letter enclosed between a pair of symbols:

$$|a\rangle, |b\rangle, |n\rangle, |x\rangle, |p\rangle, |\Psi\rangle \dots \quad (3.1)$$

#### Dirac Notation

The use of Greek letters  $\Psi$  and  $\Phi$  to denote quantum states has become a commonplace in quantum physics.

However, using Dirac notation we can denote quantum states in a variety of ways:

$$|\psi\rangle, |\phi\rangle, |0\rangle, |1\rangle, |2\rangle \dots, |a\rangle, |b\rangle \dots$$

### 3.2.3 State Content

States in classical mechanics explicitly contain a pair of values:

$$\vec{\xi} = (q, p).$$

These values are sufficient to calculate other important physical quantities, for example, total mechanical energy (using oscillator example):

$$E = \frac{kq^2}{2} + \frac{p^2}{2m},$$

---

<sup>1</sup>Dirac, P. A. M. (1939). "A new notation for quantum mechanics". Mathematical Proceedings of the Cambridge Philosophical Society. 35 (3): 416–418.

or angular momentum

$$M = qp.$$

Quantum states  $|\Psi\rangle$  contain information about quantum systems in a more sophisticated way. It is a firmly established fact, for which today exists no definite explanation.

To reveal the information contained in the state  $|\Psi\rangle$ , we must write out how  $|\Psi\rangle$  is expressed in terms of *measurable results*. More will be said about this later. For now, we just mention that if the measurable results are related to positions, the state  $|\Psi\rangle$  can be written as a function of coordinate  $q$ :

$$|\Psi\rangle \rightarrow \Psi(q).$$

Alternatively, if the measurable results are related to momentum, the state  $|\Psi\rangle$  becomes a function of momentum:

$$|\Psi\rangle \rightarrow \Psi(p).$$

### 3.2.4 Quantum State Measurement

The structure of a classical state  $\vec{\xi}$  allows us clearly see what are the values of position and momentum, from which we can calculate other important physical parameters, such as angular momentum or energy:

$$\vec{\xi} = (x, p) \quad \rightarrow \quad H = \frac{kx^2}{2} + \frac{p^2}{2m}.$$

How do we get position, momentum, energy and so on from a *quantum state*  $|\Psi\rangle$ ?

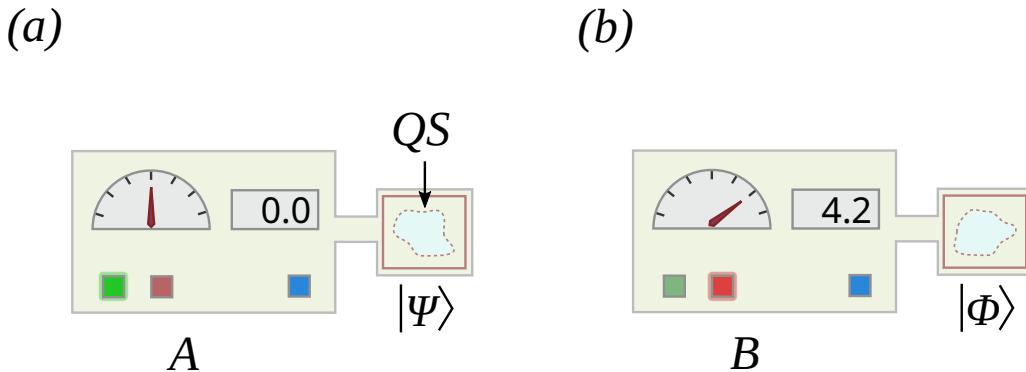


Figure 3.2: (a) Initial state of classical apparatus and quantum system (QS). (b) After the measurements, the apparatus and the quantum system might change their state.

Properties of a quantum system are revealed to us in the process of *measurement*, as illustrated in the Figure 3.2. The measurement process involves two systems: *measuring apparatus* and the *quantum system* under test.

The apparatus *interacts* with the quantum system in a certain way (e.g. by applying magnetic field, or by sending electromagnetic radiation, or by scattering electrons from it etc.) and as a result the state of the apparatus might change from  $A$  to  $B$ , and the state of the quantum system might change from  $|\Psi\rangle$  to  $|\Phi\rangle$ . It is through the observable change of the state of the apparatus that we infer the change in the state of the quantum system. Additionally, the apparatus provides us with the *value* of the parameter being measured, indicating it as a number on a screen, or as the number on a scale. We can express this fact symbolically as follows:

$$A, |\Psi\rangle \xrightarrow{\hat{M}} B, |\Phi\rangle; \quad (3.2)$$

here  $\hat{M}$  is the *measurement operator*.

The measuring apparatus is a *classical device* – usually large – compared to quantum systems such as atoms, molecules, or small crystals – and operating in accordance with the laws of classical physics: classical mechanics, classical electrodynamics, classical optics and so on. It is important to understand the importance of the measuring apparatus in quantum physics. Although quantum physics focuses on quantum effects, the classical measuring apparatus is always implicitly present in quantum theory. The mathematical tools of linear algebra, such as vectors and operators, provide a convenient language to express this fact.

### 3.2.5 Proper States

In general, measurement process  $\hat{M}$  changes the state of classical apparatus and changes the state of quantum system being measured. We expressed this symbolically as follows:

$$A, |\Psi\rangle \xrightarrow{\hat{M}} B, |\Phi\rangle. \quad (3.3)$$

In certain important cases the initial state of the apparatus, the initial state of the quantum system, and the measurement process are so “aligned” that no change of states happens:

$$A, |\Psi\rangle \xrightarrow{\hat{M}} A, |\Psi\rangle. \quad (3.4)$$

In this case the quantum state  $|\Psi\rangle$  is considered a special state relative to the measurement  $\hat{M}$  and is called its *proper state*; German word *eigen* is also often used instead of “proper”, thus *eigen state*. Obviously, if a quantum system is in a proper state of  $\hat{M}$ , then repeated measurements of the quantity  $\hat{M}$  will yield the same results over and over again:

$$A, |\Psi\rangle \xrightarrow{\hat{M}} A, |\Psi\rangle \xrightarrow{\hat{M}} A, |\Psi\rangle \xrightarrow{\hat{M}} \dots \quad (3.5)$$

A comparative illustration of proper states and general states is shown in the Figure 3.3.

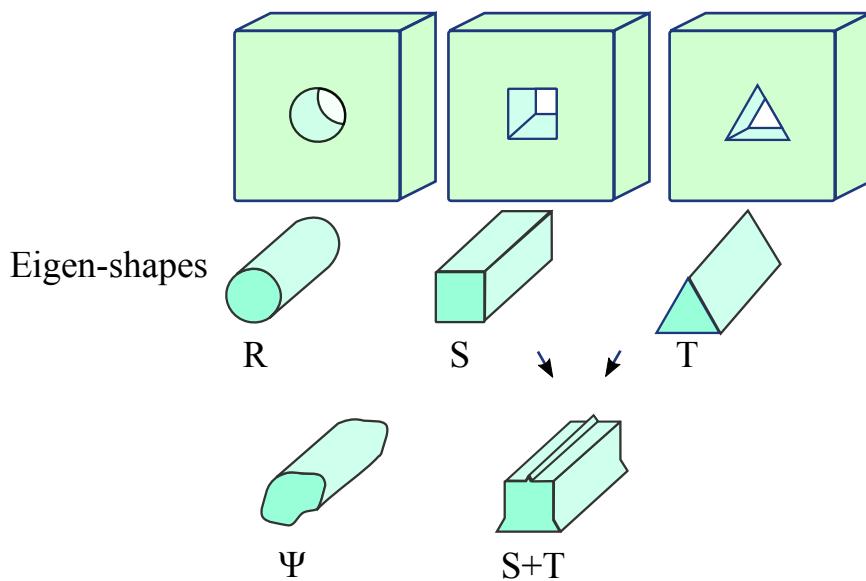


Figure 3.3: Measurement procedure can be compared to a special form that takes a malleable “state”  $\Psi$  and produces an eigen-shape.

### 3.2.6 Eigen-Value Problem

A special notation is used to describe the process of measurement on proper states. Instead of the relation

$$A, |\Psi\rangle \xrightarrow{\widehat{M}} A, |\Psi\rangle$$

the following, more compact, equation is written:

$$\widehat{M}|\Psi\rangle = A|\Psi\rangle. \quad (3.6)$$

At this point we can not rigorously justify such an equation, because we don't know what it means to multiply a quantum state  $|\Psi\rangle$  by a number  $A$  – the reading of a classical measuring instrument. We don't yet have either graphical or algebraic representation for quantum states. Nevertheless, we can appreciate what the equation (3.6) expresses: *As the result of the measurement of quantity  $\widehat{M}$ , the state of the quantum system  $|\Psi\rangle$  remains unchanged, and the measured value is reported by the classical apparatus as a number  $A$ .*

As stated above, the state  $|\Psi\rangle$  is a proper state of the measurement operation  $\widehat{M}$ . The corresponding value  $A$  is called *proper value* or *eigen-value* for the state  $|\Psi\rangle$ . The equation (3.6) provides mathematical formulation of a problem of determining all possible proper states and proper values for a given measurement operation  $\widehat{M}$ . Such a mathematical problem is called *eigen-value problem*.

Eigen-value problem is not limited to quantum physics, it is encountered in many branches of physics and

mathematics.

### 3.2.7 Probability

For a given measurement operation  $\widehat{M}$  an arbitrary state  $|\Psi\rangle$  is *not* its proper state. When the measurement is performed, the states of both the quantum system and the classical apparatus change, as expressed by the relations:

$$A, |\Psi\rangle \xrightarrow{\widehat{M}} B, |\Phi\rangle.$$

This relation is incomplete as it does not reflect a *fundamental fact of randomness* which is essential to quantum world. What is observed in experiments, is the following: Given initial state  $|\Psi\rangle$  of quantum system, the result of the measurement operation  $\widehat{M}$  can, in general, be one of many outcomes:

$$A, |\Psi\rangle \xrightarrow{\widehat{M}} \begin{cases} B, |\Phi\rangle & \text{in } N_1 \text{ cases out of } N. \\ C, |X\rangle & \text{in } N_2 \text{ cases out of } N. \\ \dots & \dots \\ D, |\Upsilon\rangle & \text{in } N_k \text{ cases out of } N. \end{cases}$$

In other words, the *probability* of measuring the value  $B$  is

$$p_1 = \frac{N_1}{N}.$$

Similarly, the probability of measuring the value  $C$  is

$$p_2 = \frac{N_2}{N}$$

and so on. It should be clear that each probability is non-negative and less than unity:

$$0 \leq p_k \leq 1.$$

Such random branching of results underlines the fact that general state  $|\Psi\rangle$  is *not “aligned”* with the apparatus and the measurement  $\widehat{M}$ : There is no guaranteed result of a single measurement, and *no definite* value of the physical quantity corresponding to the measurement procedure  $\widehat{M}$ . In simpler language: Quantum system may be in a state with no definite value of position, or no definite value of momentum, or no definite value of energy,

for example.

### 3.2.8 Superposition

It is an experimental fact that measurement  $\hat{M}$  performed on a quantum system in a state  $|\Psi\rangle$  will – in general – yield random results each time the measurement is performed. We express this symbolically as follows:

$$A, |\Psi\rangle \xrightarrow{\hat{M}} \begin{cases} p_1, |\Phi_1\rangle, V_1 \\ p_2, |\Phi_2\rangle, V_2 \\ \dots \\ p_n, |\Phi_n\rangle, V_n \end{cases}$$

Here the possible results (states of classical apparatus) are denoted by the values  $V_k$ , corresponding final states of the quantum system are denoted by  $|\Phi_k\rangle$ , and the respective probabilities are  $p_k$ .

We will set aside the question of the nature of the states  $|\Phi_k\rangle$  for a moment. Instead, let's think how quantum state  $|\Psi\rangle$  can “evolve” into the state  $|\Phi_k\rangle$  with probability  $p_k$ ? And how this fact can be mathematically represented?

We can state quite generally that the state  $|\Psi\rangle$  is some function of the states  $|\Phi_k\rangle$  and respective probabilities  $p_k$ :

$$|\Psi\rangle = F(|\Phi_1\rangle, |\Phi_1\rangle, \dots, |\Phi_1\rangle, p_1, p_2, \dots, p_n),$$

or more compactly

$$|\Psi\rangle = F(|\Phi_k\rangle, p_k) \quad k = 1, 2, \dots, n.$$

Now the states  $|\Psi\rangle$  and  $|\Phi_k\rangle$  are of the same nature: they are different states of the *same quantum system*. There should be no fundamental difference in how they are treated mathematically.

To see how one mathematical object can be constructed from other mathematical objects of similar nature, we can turn to arrow-vectors for an example. In planar geometry we can have a vector  $\vec{\psi}$  which is “made of” other vectors:

$$\vec{\psi} = c_1 \vec{\phi}_1 + c_2 \vec{\phi}_2.$$

For problems that require more dimensions, similar *decomposition* can be written:

$$\vec{\psi} = c_1 \vec{\phi}_1 + c_2 \vec{\phi}_2 + \dots + c_n \vec{\phi}_n.$$

This expression is understood as follows: the vector  $\vec{\psi}$  is aligned with each vector  $\vec{\phi}_k$  to a certain degree; the “degree of alignment” is given by the coefficient  $c_k$ .

In a manner similar to arrow-vectors, we could at least tentatively write

$$|\Psi\rangle = p_1|\Phi_1\rangle + p_2|\Phi_2\rangle + \dots p_n|\Phi_n\rangle. \quad (3.7)$$

Mathematically, this is the simplest way to write the state  $|\Psi\rangle$  as the function of the states  $|\Phi_k\rangle$  and respective probabilities  $p_k$ . To use this approach we must understand what it means to multiply a state by a number (e.g.  $p_1|\Phi_1\rangle$ ), and what it means to add two states together.

The expression (3.7) is called *superposition* of states. Such expressions are common to all physical theories that use so called *linear equations* that describe state evolutions; more on this later. The superposition assumption (3.7) is a good starting point, but it does not capture all properties of quantum states. We will see how to improve this situation below.

### 3.2.9 States Overlap

Given quantum states  $|\Psi\rangle$  and  $|\Phi\rangle$  we can ask: How different are they? To answer this question we need some *measure of likeness*<sup>2</sup> of a pair of states. That is to say: We need a function (operator) that takes two states and produces a number that quantifies the similarity (or difference) between the states:

$$\hat{\sigma}|\Psi\rangle|\Phi\rangle = w,$$

where  $w$  is some number.

$$\boxed{\hat{\sigma}|\Psi\rangle|\Psi\rangle = 1, \quad (100\%).} \quad (3.8)$$

Thorough analyses of physically possible measurements indicate that quantum states *can not* be written as functions of both positions and momentum. Measuring position of a quantum object affects its momentum, and, analogously, measuring momentum affects the position. Precise measurement of both is impossible, thus, no representation of quantum state exists in terms of functions

$$|\Psi\rangle \rightarrow \Psi(q, p).$$

In contrast to the classical state  $\vec{\xi} = (q, p)$ , no state exist in the form of  $|q, p\rangle$ .

---

<sup>2</sup>Or the measure of difference.

### 3.3 Quantum Dynamics

The state of a classical system evolves with time according to the equations of classical dynamics. In Hamiltonian approach these equations are Hamiltonian equations of motion. The state of a quantum system evolves with time according to the equations of *quantum dynamics*. One such equation is Schrödinger's equation:

$$i\hbar\partial_t|\Psi\rangle = H|\Psi\rangle.$$

$$|a\rangle, |b\rangle, |n\rangle, |x\rangle, |p\rangle, |\Psi\rangle \dots \quad (3.9)$$

#### State Vectors

Schrödinger's equation requires quantum state to be a vector. Indeed, its left-hand side reads

$$i\hbar\partial_t|\Psi\rangle = \frac{i\hbar}{\delta t} (|\Psi(t + \delta t)\rangle - |\Psi(t)\rangle).$$

Thus, we must be able to add/subtract states and multiply them by numbers.

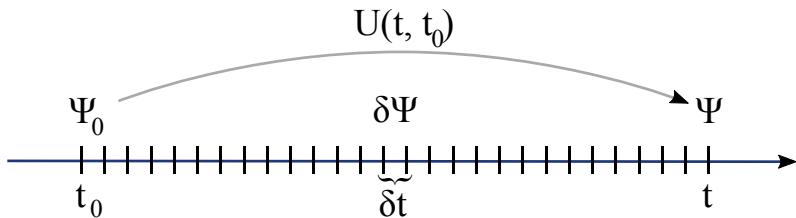


Figure 3.4: State of a system changes in time. Mathematical description of the evolution is given by an evolution equation involving evolution operator which is determined by the Hamiltonian of the system.

Starting with initial state  $|\Psi_0\rangle$  at  $t = t_0$ , we can find the state at a later moment of time  $t_1 = t_0 + \delta t$ :

$$|\Psi_1\rangle = |\Psi_0\rangle + \frac{\delta t}{i\hbar} H |\Psi_0\rangle.$$

Advancing further, we can calculate the state at even later time  $t_2 = t_1 + \delta t$ :

$$|\Psi_2\rangle = |\Psi_1\rangle + \frac{\delta t}{i\hbar} H |\Psi_1\rangle.$$

In general, given the state  $|\Psi_n\rangle$  at time  $t_n$ , we can find the state at a later time  $t_n + \delta t$ :

$$|\Psi_{n+1}\rangle = |\Psi_n\rangle + \frac{\delta t}{i\hbar} H |\Psi_n\rangle.$$

An important observation can be made. First, using the trivial *unit operator*  $I$ :

$$I|\Psi_n\rangle = |\Psi_n\rangle,$$

we can write

$$|\Psi_{n+1}\rangle = \left( I + \frac{\delta t}{i\hbar} H \right) |\Psi_n\rangle.$$

Second, the change of the state from  $|\Psi_0\rangle$  at time  $t_0$  to  $|\Psi_n\rangle$  at time  $t_n$  can be done by composing  $n$  steps, each step advancing the state according to the formulas given above. Using the fact that

$$\delta t = \frac{t_n - t_0}{n} = \frac{t}{n},$$

we can write

$$|\Psi_n\rangle = U(t_{n-1}) \cdots U(t_1)U(t_0)|\Psi_0\rangle,$$

where

$$U(t_k) = I + \frac{\delta t}{i\hbar} H(t_k).$$

For a quantum system with time-independent Hamiltonian  $H$ , the operator  $U$  is also time-independent and the evolution of the state reduces to

$$|\Psi_n\rangle = \left( I + \frac{t}{in\hbar} H \right)^n |\Psi_0\rangle.$$

Using the limit of vanishingly small steps  $\delta t \rightarrow 0$  (implying the limit  $n \rightarrow \infty$ ) we finally obtain

$$|\Psi_n\rangle = e^{\frac{tH}{i\hbar}} |\Psi_0\rangle. \quad (3.10)$$

The preceding manipulations are purely mathematical, they describe a formal scheme for deducing some quantity  $|\Psi\rangle$  at time  $t$ , given its value  $|\Psi_0\rangle$  at time  $t_0$ . To fill this scheme with a physical content we must do the following:

- Provide physical meaning to the operator  $H$
- Describe how the operator  $H$  acts on any state  $|\Psi\rangle$ , or
- Describe how the operator  $H$  acts on some *basic* states  $|b_1\rangle, |b_2\rangle, |b_3\rangle$  etc.; and then

- Determine how an arbitrary state  $|\Psi\rangle$  can be “built from” those *basic states*:

$$|\Psi\rangle = c_1|b_1\rangle + c_2|b_2\rangle + c_3|b_3\rangle + \dots$$

### 3.4 Quantum Hamiltonian

In quantum physics Hamiltonian approach is at the center of virtually all methods of analysis of quantum phenomena.

### 3.5 Quantum Oscillator

To arrive at the expression for quantum Hamiltonian for oscillator, we will use the method of phase space, combined with the quantization of action.

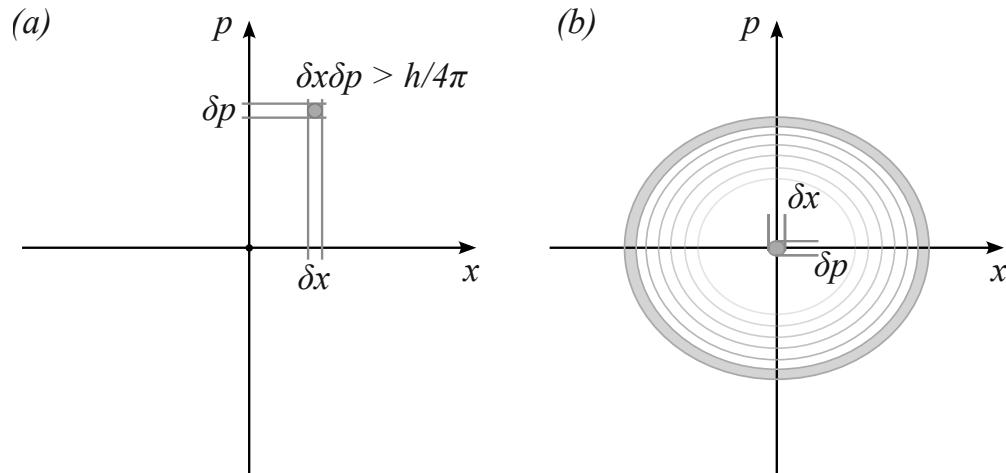


Figure 3.5: (a) Heisenberg uncertainty implies that the state  $(x, p)$  of a system can not be known precisely. (b) When an oscillator absorbs energy and changes state, the area of the phase-space figure changes by a quantized amount proportional to the quantum of action  $h$ .

The area of the figure defined by the oscillator “trajectory” is  $A = \pi x_m p_m$ , where  $x_m$  is the maximum value of the position, and  $p_m$  is the maximum value of the momentum. Using the dimensionless units, this becomes:

$$A = \pi x_e p_e \bar{x}_m \bar{p}_m = \pi x_e p_e \bar{H} = \pi x_e p_e \frac{H}{H_e}.$$

The frequency of the oscillator is related to  $x_e$ ,  $p_e$  and  $H_e$ :

$$\omega = \frac{2H_e}{x_e p_e},$$

which leads to

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

The quantization of action implies that  $\Delta A = h$ , leading to

$$\Delta H = \frac{\hbar\omega}{2\pi} = \hbar\omega.$$

Therefore, the energy of the oscillator is

$$H_n = n\hbar\omega + H_0,$$

where  $H_0$  is the lowest energy of an oscillator. It is the energy of the oscillator in its most “compact” state when  $x_m$  and  $p_m$  are minimal.

The smallest area of the phase space is determined by the Heisenberg uncertainty principle

$$\delta x \delta p > \frac{\hbar}{4\pi}.$$

The area of the phase space for the smallest action is

$$A_0 = \pi(\delta x/2)(\delta p/2) > h$$

implying that the minimal energy of the oscillator is

$$H_0 = \frac{A_0\omega}{2\pi} =$$

### 3.6 Parts and Whole\*

**Keywords:** *Joint systems (composite systems), joint states, joint dynamics, joint measurements.*

Whole is an aggregate of *connected* parts.

We already met several examples of *composite* physical systems that have *structure* and *parts*. Harmonic oscillator consists of a body and a spring, and an immovable “wall” that the spring is attached to. However, we only focused on the motion of the body, specifying its position  $x$  and momentum  $p$ . When studying the simplest atom – hydrogen atom – we will be dealing with a kind of *three body problem* where an electron, a proton, and

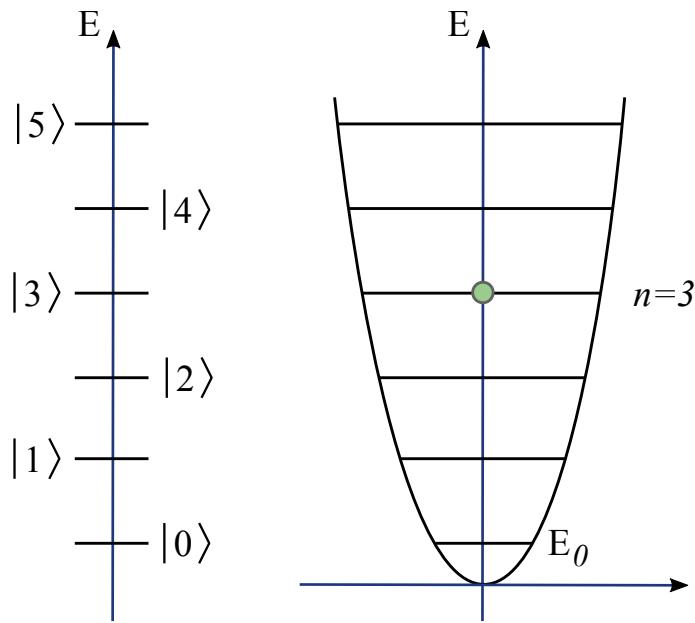


Figure 3.6: Energy of different states of quantum oscillator are separated from each other by the same amount  $h\nu = \hbar\omega$ . The lowest possible energy is not zero,  $E_0 = H_0 > 0$ .

electromagnetic field will constitute a single quantum system called atom.

Thus, simple, isolated quantum systems are idealization and are rarely of practical interest. It is important to know how to treat systems with many parts and how those parts interact to make the system behave as one whole. Both classical and quantum physics have a way to treat composite systems (see Figure 3.7).

$$|\Psi\rangle = |A\rangle \otimes |B\rangle .$$

### 3.6.1 Important Composite States

Quantum science and technology gradually expand the boundaries of experiments and applications. More and more complicated systems, involving ever increasing number of parts, are studied. We will review several important examples in this section.

#### Two Photon States

$$\Psi = \frac{1}{\sqrt{2}} (|0\rangle \otimes |2\rangle + |2\rangle \otimes |0\rangle) .$$

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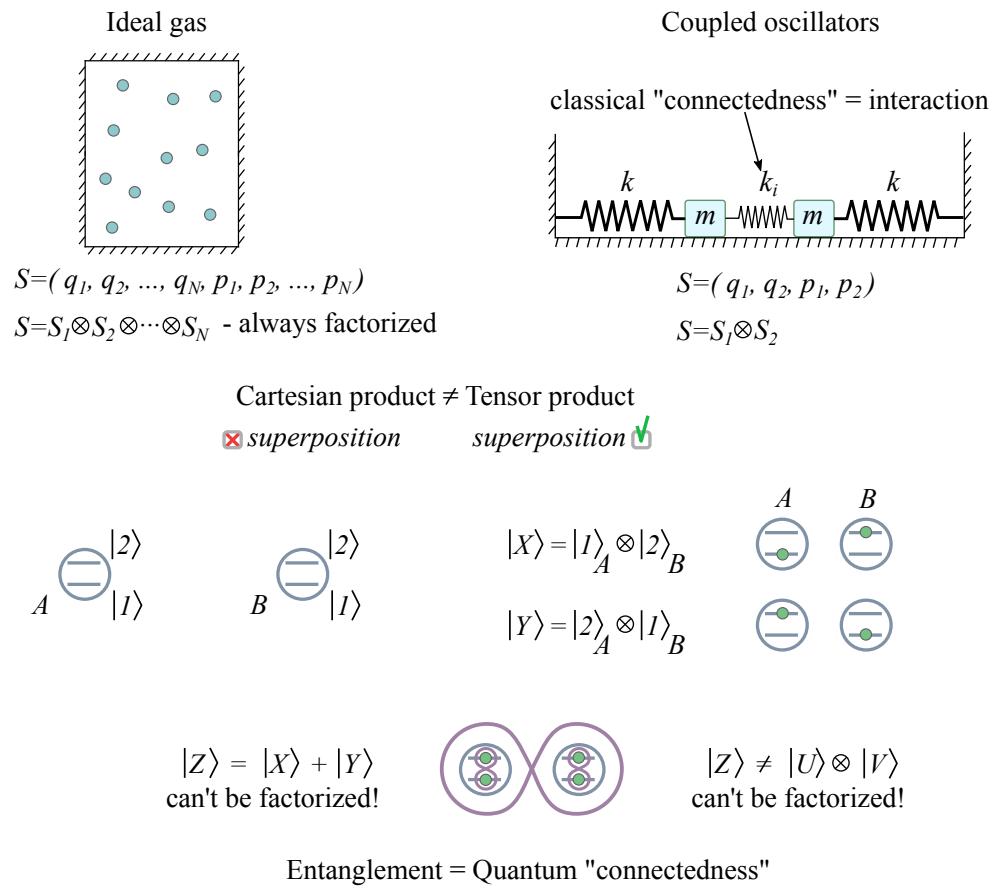


Figure 3.7: Descriptions of composite systems in classical and quantum physics have both similarities and differences.

**Bell States**

**GHZ State**

**Superconducting State\***

**Qat States**

Consider a large quantum system with microscopical number of parts. Let's call it *qat* – for quantum cat. Assuming each part of qat is a qubit, the two extreme states of the cat can written as follows:

$$|A\rangle = |1\rangle \otimes |1\rangle \otimes |1\rangle \cdots \otimes |1\rangle \quad \text{and} \quad |D\rangle = |2\rangle \otimes |2\rangle \otimes |2\rangle \cdots \otimes |2\rangle .$$

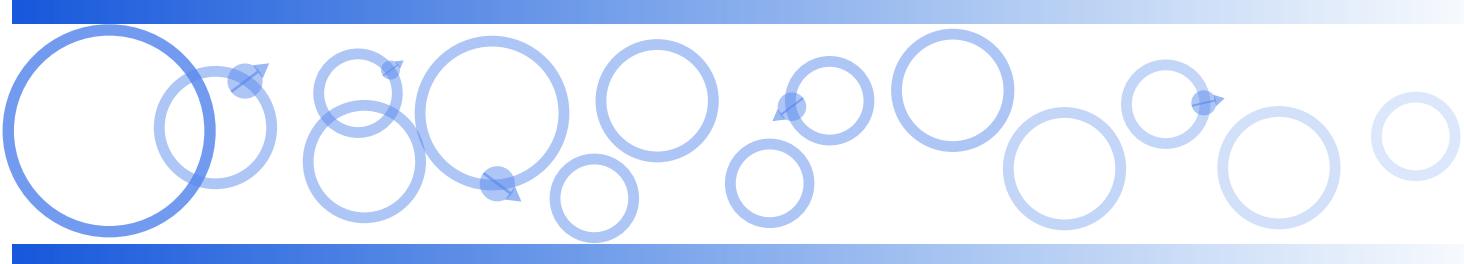
Of course, other states are possible:

$$|B\rangle = |1\rangle \otimes |2\rangle \otimes |1\rangle \cdots \otimes |1\rangle \quad \text{and} \quad |C\rangle = |2\rangle \otimes |1\rangle \otimes |2\rangle \cdots \otimes |2\rangle ,$$

and many more of this kind, as well as superpositions of these various product states. Namely, quantum physics allows the state

$$|\Psi\rangle = |A\rangle + |D\rangle .$$

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## 4. Quantum Fields

In physics and mathematics a *field* is defined as a *value assigned to each point of space*. The exact nature of value depends on the type of a field (*scalar, vector, tensor, spinor fields*).

To better understand the nature of quantum fields, it is important to know fields are treated in classical physics.

### 4.1 Classical Field

In classical physics *field* is a physical entity extended over a region space (finite or infinite). Electricity and magnetism provide excellent examples of a physical field – electric field  $\vec{E}$  and magnetic field  $\vec{H}$ .

Take for example a charged object. It affects motion of other charged objects in its vicinity without getting in *direct contact* with them. The interaction is *mediated* by an *electrostatic field* created by the charged object. The Figure 4.1(a) shows a charge  $Q$  “surrounded” by a static electric field. It also shows that any other charge is being “forced” to move either towards or away the charge  $Q$ . In this example the charge  $q$  is being pulled towards  $Q$ . To simplify the picture, the field due to the charge  $q$  is not shown.

In the Figure 4.1(b) a wire carrying current  $I$  is shown. The current produces static magnetic field everywhere around the wire; for simplicity only three horizontal “slices” are shown. The magnetostatic field of the current affects the motion of charged particles and may affect orientations of other magnetic particles.

The electric and magnetic fields were introduced into physics by Michael Faraday.

#### Electromagnetic Field

Is electromagnetic field *scalar* or *vector* field? In classical electromagnetism it is neither. Electromagnetic field is *tensor field*. Electrostatic or magnetostatic experiments reveal the nature of electromagnetic field only partially, creating an impression that it is a combination of two separate vector fields – electric and magnetic fields.

##### 4.1.1 State Of Field

To specify the *state of a field* we must give the value for the field at each point of space. In other words, we must specify a function  $\tilde{F}(x)$  for every point of space  $x$ . The value  $\tilde{F}$  can be a number (scalar field), a vector (vector

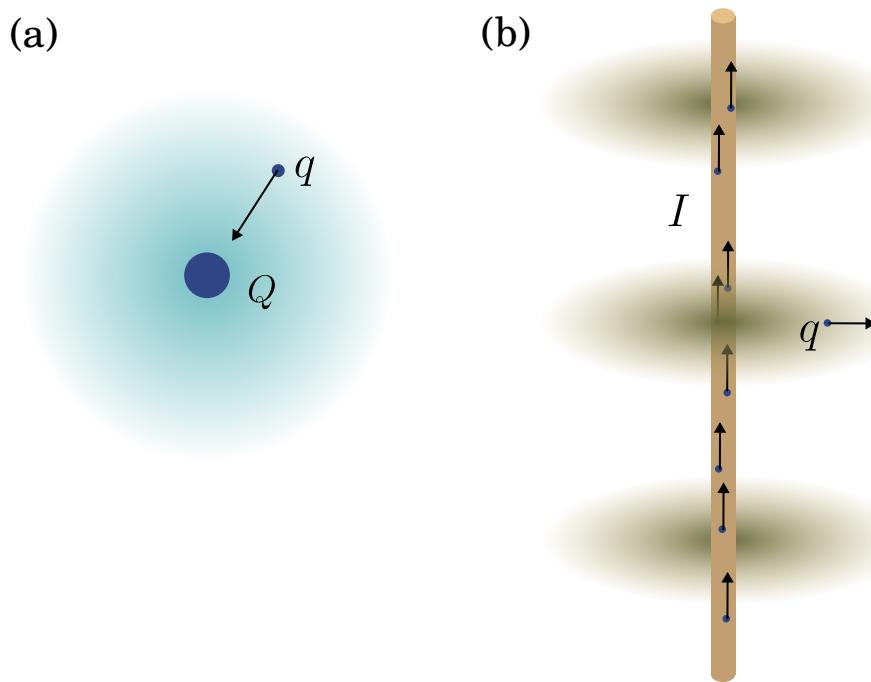


Figure 4.1: (a) Electrostatic field. (b) Magnetostatic field.

field), tensor (tensor fields), spinor (spinor field). For example, an electrostatic field around a point-like charge  $Q$  can be described using *vector field* which assigns an electric field vector  $\vec{E}$  for each point  $P$  around the charge.

One important property of many classical fields and equations that describe their dynamics is expressed by the *principle of superposition*. (One important exception from this principle is the gravitational field.)

#### 4.1.2 Superposition

Electromagnetic field and equations that describe its motion have a very important property called *linearity*. It means that when dealing with several charges (several sources of the field) the total field can be found by simple addition of fields from each source. Such “adding up” of fields is called *superposition*. See Figure 4.4 for illustration.

#### 4.1.3 Vacuum

The concept of vacuum has different interpretation in different areas of physics. Naively, vacuum is the absence of everything (particles and fields) in a given region of space. Absolute vacuum – total absence of particle and fields – is an idealization. In practice, physicist try to achieve different *levels of vacuum*: from high to ultra-high; see Figure 4.5.

#### 4.1.4 Mechanics of Fields

Starting with simple mechanical system, such as an oscillator, we can build more complicated, extended systems with many more *degrees of freedom*. The idea is illustrated in the Figures 4.6 and 4.7.

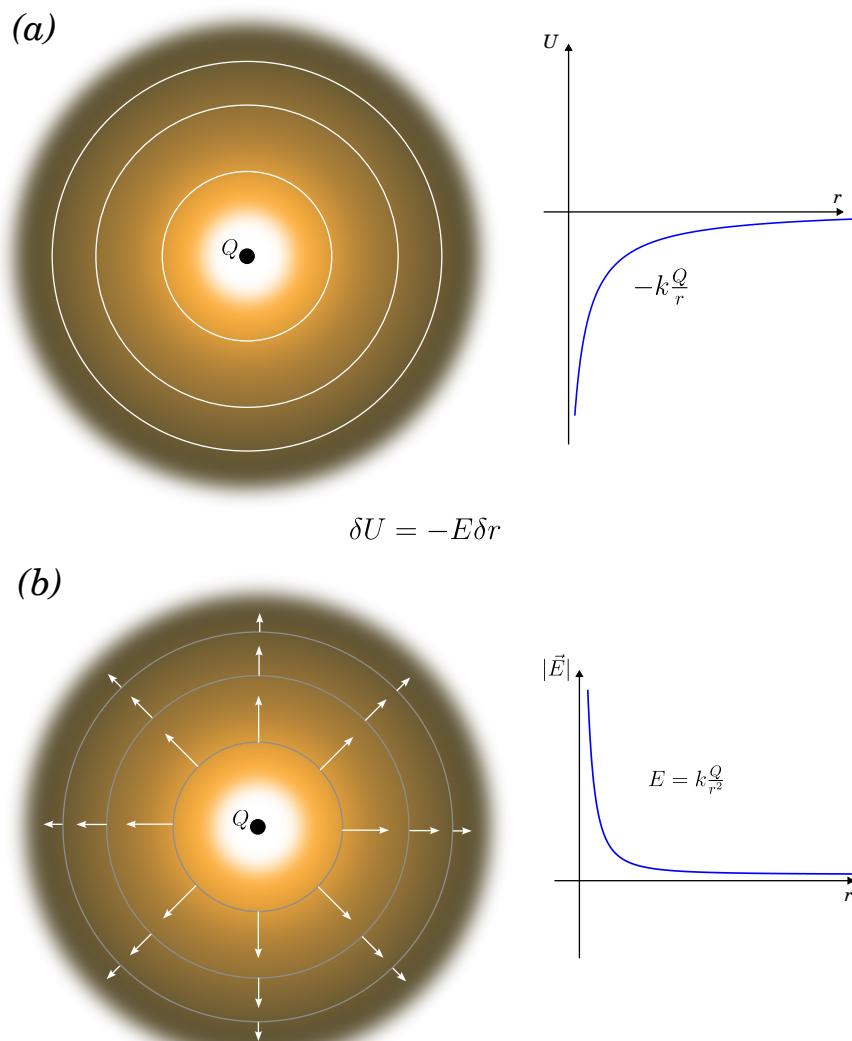


Figure 4.2: (a) Electrostatic field potential  $U$ . (b) Electrostatic field strength vector  $\vec{E}$ .

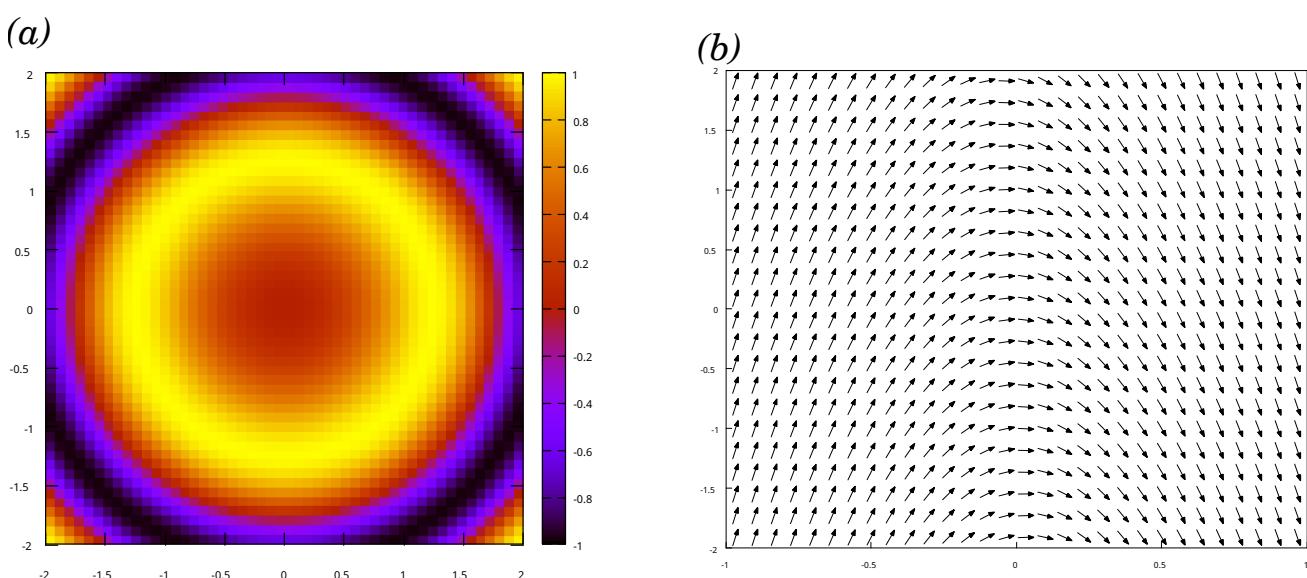


Figure 4.3: (a) Scalar field – number assigned to each point in space. (b) Vector field – vector assigned to each point in space.

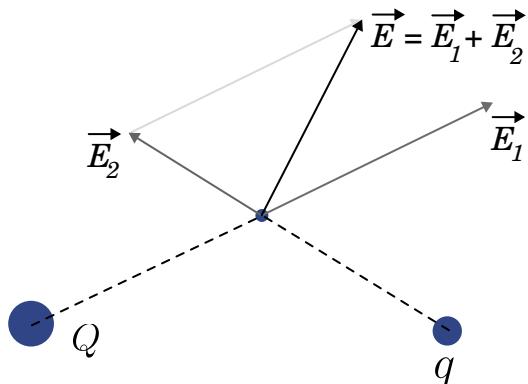


Figure 4.4: Electromagnetic fields from several sources simply add up.

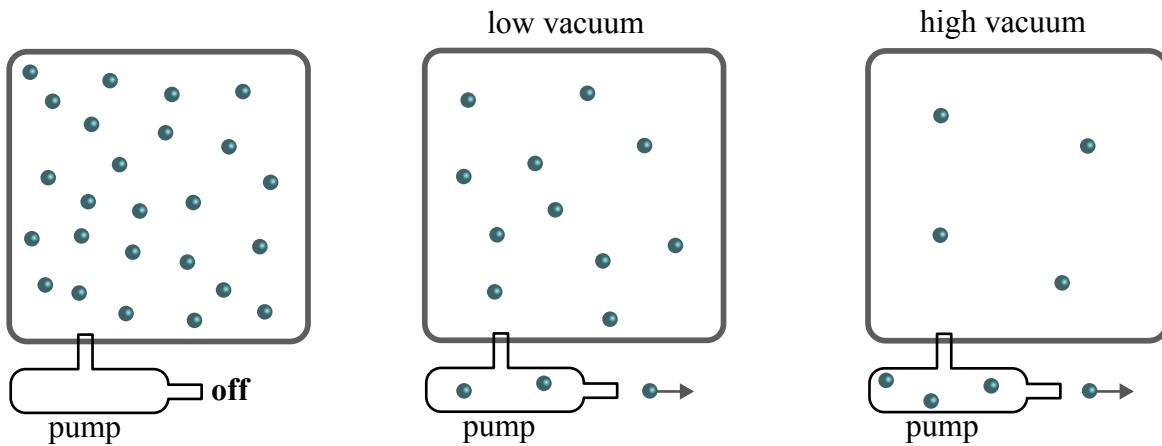


Figure 4.5: Different levels of vacuum. Absolute vacuum – total absence of undesired elements – is not achievable.

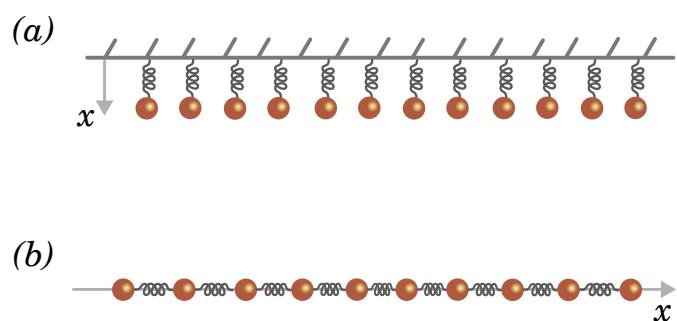


Figure 4.6: (a) Not coupled and (b) coupled oscillators.

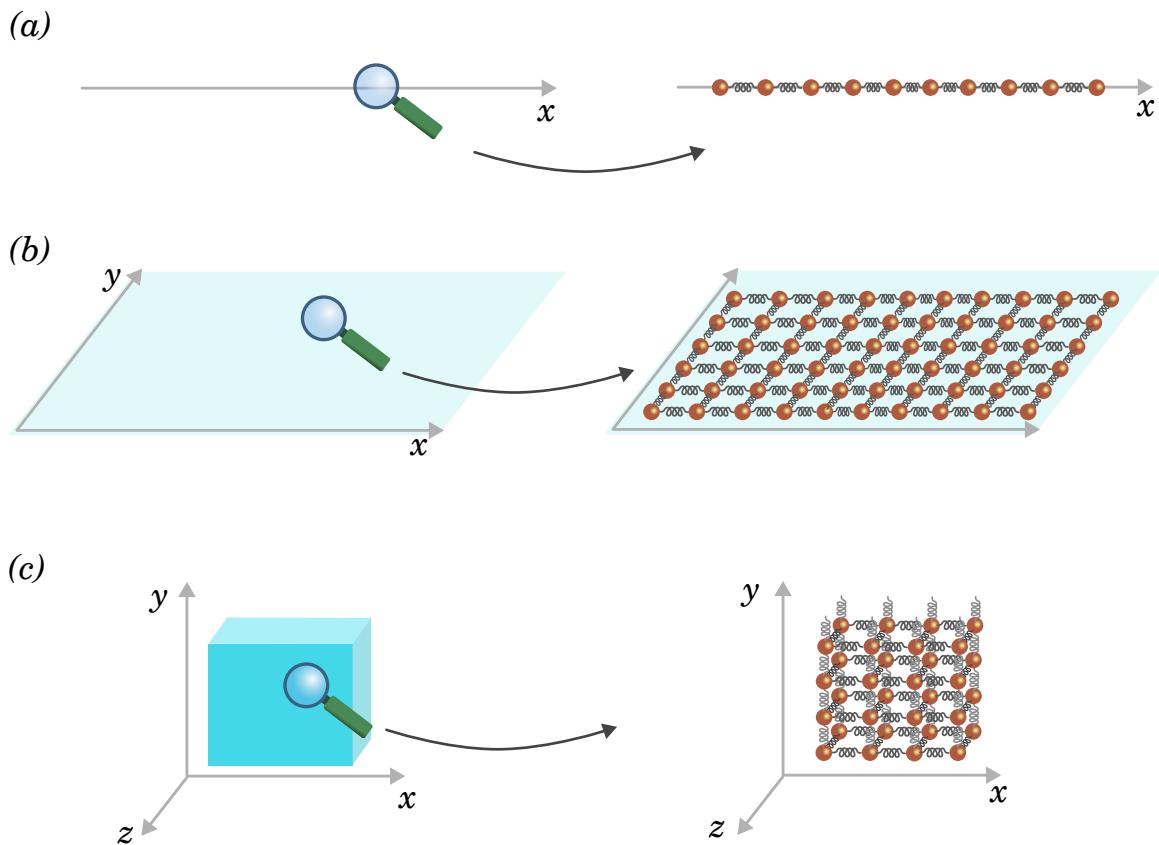


Figure 4.7: Field as a mechanical system with infinite (but countable) number of degrees of freedom.

When we imagine the size of each “oscillator” getting ever smaller, and the number of such oscillators getting ever larger, with the total system filling the whole space, we will arrive at a simple yet powerful model of a field.

Kinetic energy per unit “volume”:

$$\epsilon_k = \frac{\mu\nu^2}{2},$$

where  $\nu = \partial_t \phi$  is the field’s “velocity”.

Potential energy per unit “volume”:

$$\epsilon_p = \frac{\kappa\phi^2}{2}.$$

Therefore, we can write Lagrangian of a scalar field  $\phi(x)$  as follows:

$$\mathcal{L} = \frac{\mu(\partial_t \phi)^2}{2} - \frac{\kappa\phi^2}{2}.$$

### 4.1.5 Waves

Field excitations can propagate in space with time. In this case we are talking about *traveling waves*. Excitations can be “trapped” inside a certain region/volume/domain/cavity. In this case we might observe *standing waves*.

Mathematical description of traveling and standing waves is based on the periodic (trigonometric) functions.

#### Electromagnetic Waves

Electromagnetic radiation is emitted whenever a charged particle(s) experiences acceleration. Accelerated object (charge) changes its kinetic energy, either loosing or absorbing energy from another source – electromagnetic field.

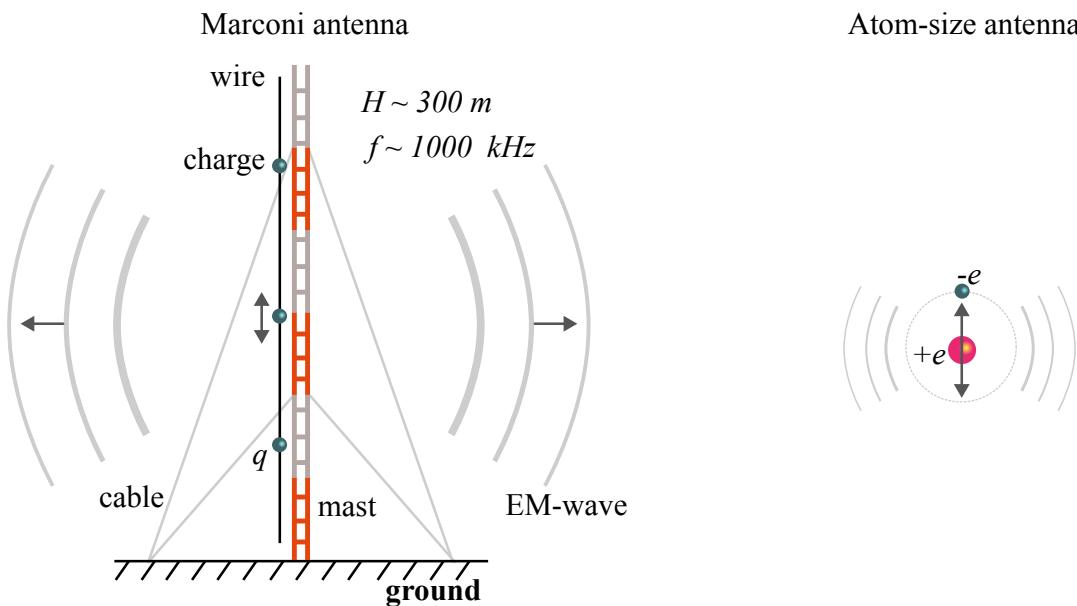


Figure 4.8: Charges moving periodically back and forth will create periodic electromagnetic field which travels away from the source as electromagnetic wave. The same process should occur in classical model of an atom.

A periodically accelerated charge, for example a charged body attached to a spring, will emit electromagnetic radiation of periodic nature. This is the idea behind an antenna, where charges in a wire are pushed and pulled back and forth to produce electromagnetic radiation in a form of a wave. In classical electromagnetism, the frequency of the electromagnetic wave is determined by the frequency of the periodic motion of the charged body. When applied to the simplest atom – hydrogen atom – this logic fails to explain observed atomic phenomena, such as the stability of atoms and the spectra of radiation emitted by hydrogen atoms. In the next chapter we will learn how to describe such phenomena using quantum framework.

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## 4.2 Quantum Field

Quantum physics describes fields as the set of quantum oscillators, as illustrated in the Figure 4.9.

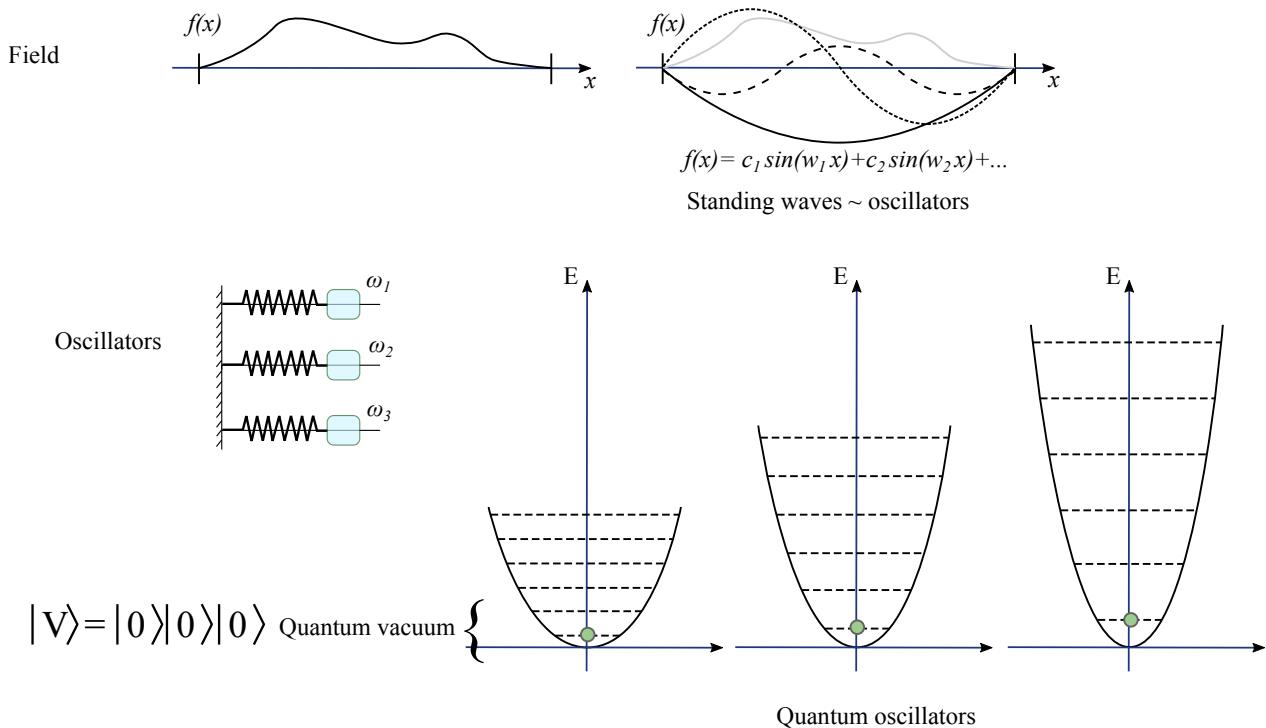


Figure 4.9: Fields can be described as functions over space  $f(x)$ . Such functions can be expressed as the sum over standing waves (Fourier series), each standing wave mathematically equivalent to an oscillator. Quantum oscillators correspond to quantum description of the field.

#### 4.2.1 Quantum Vacua

Quantum vacuum is the state of a quantum field with the lowest energy. Since there exist different kinds of fields (e.g., electromagnetic, gravitational, strong, electron-positron), there are different kinds of vacua. Electromagnetic vacuum is the most well-studied.

In the picture where fields are represented as the sum of oscillators, quantum vacuum corresponds to the collection of quantum oscillators in their lowest states, with no excitation quanta (particles) present.

### 4.3 Beables, Phandles, and Events

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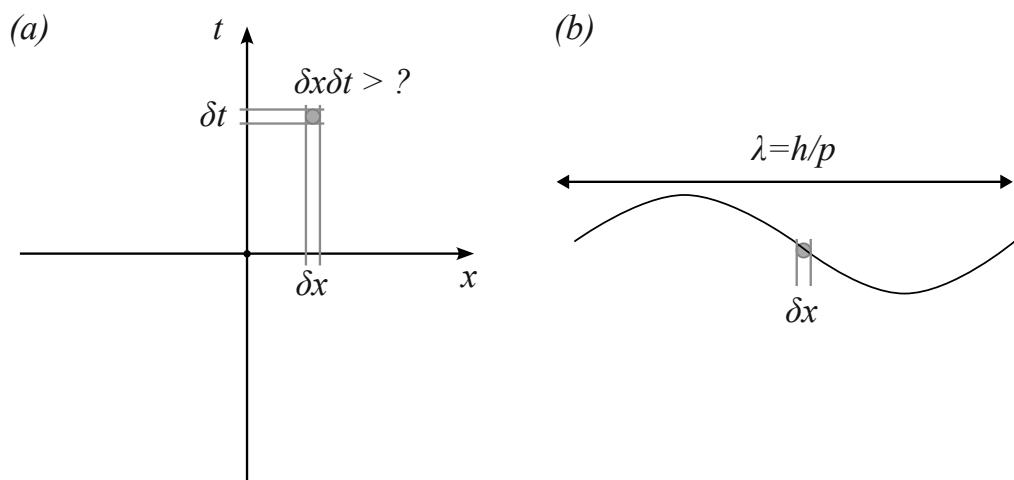
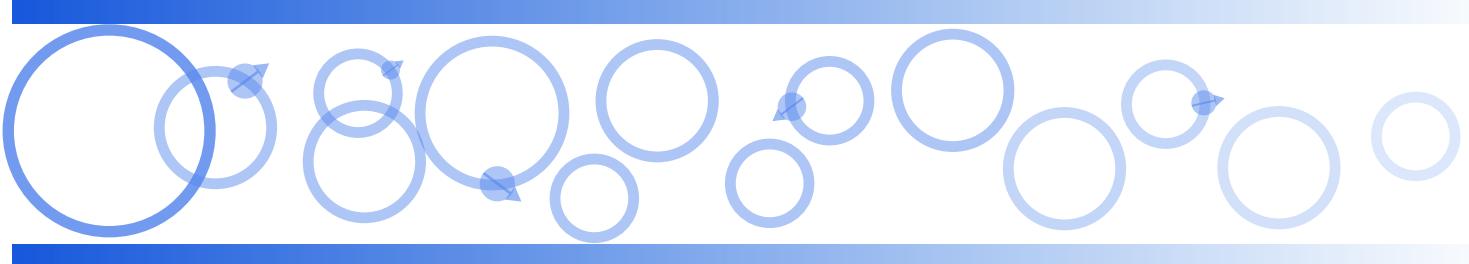


Figure 4.10: (a) In spacetime picture reality is given us through events. (b) Interacting with the world we encounter “quantum bundles” – energy pieces highly localized in time and space, but also possessing phase (and consequently wavelength  $\lambda$ ).



## 5. Quantum Phenomena

### 5.1 Atomic and Molecular Spectra

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

#### 5.1.1 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 a 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:

$$d_H \approx 1 \text{ \AA} \quad \text{\AAngstrom} = 10^{-10} (m).$$

#### \* 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.

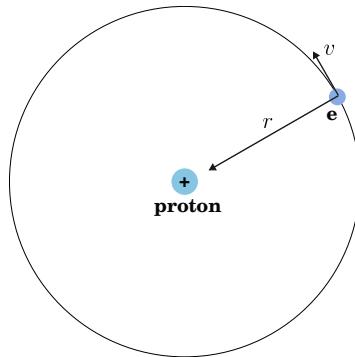


Figure 5.1: Planetary model of hydrogen atom.

### 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 5.1.

The circular motion of the electron around the nucleus is mathematically 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

$$k = \frac{1}{4\pi\epsilon_0}.$$

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

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

Using de Broglie hypothesis about the relation between momentum and wavelength

$$p\lambda = h,$$

and combining it with *quantization hypothesis*:

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

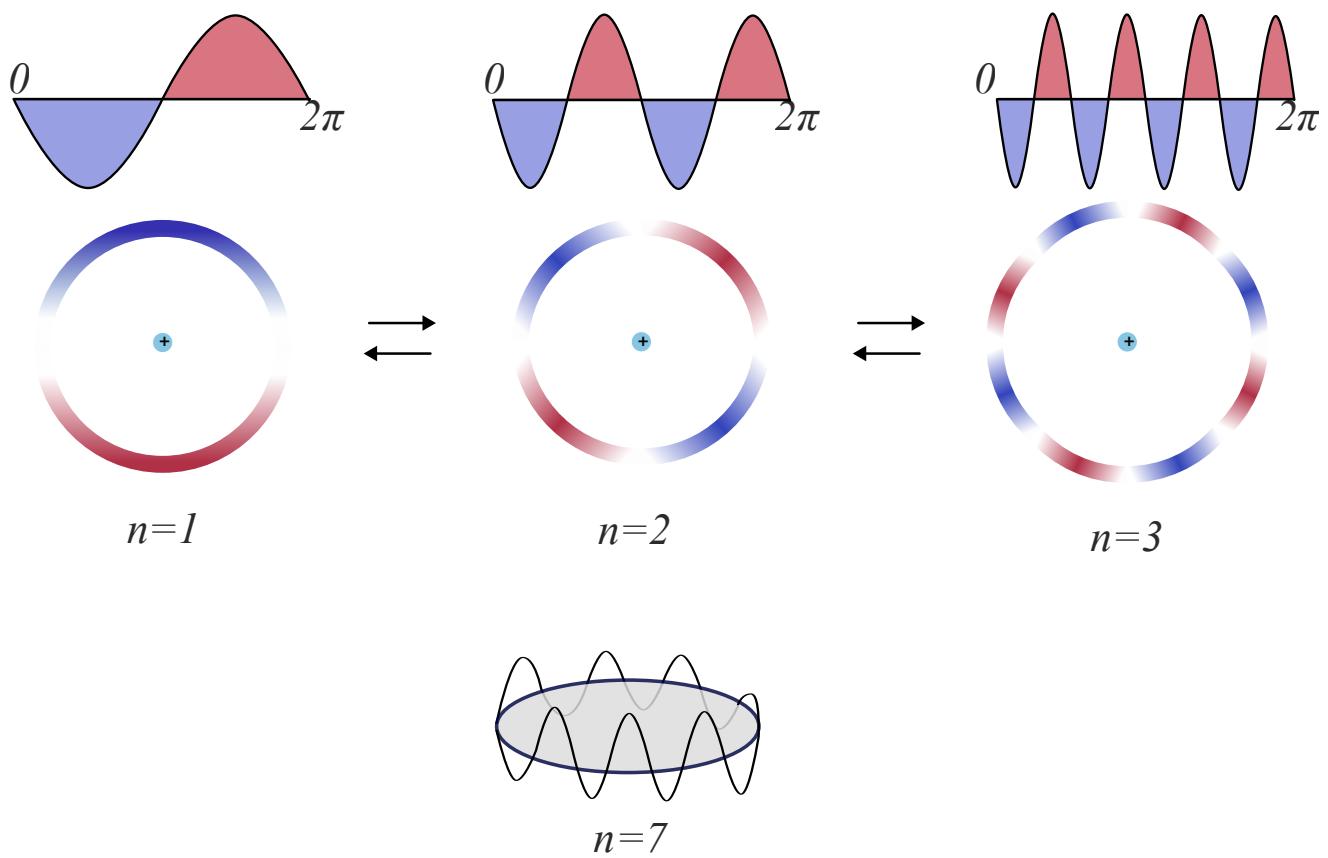


Figure 5.2: Orbits allowed by the semi-quantum model.

or, equivalently,

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

we find possible solutions for the radius of the “orbit”:

$$r_n = \frac{\hbar^2 n^2}{km_e q_e^2} \quad n = 1, 2, 3, \dots$$

The smallest value of the radius is

$$a_0 = r_1 = \frac{4\pi\varepsilon_0\hbar^2}{m_e q_e^2} = 0.523 \text{ \AA}.$$

It is called *Bohr radius*. Thus, the smallest diameter of electron’s orbit is about 1 Ångstrom.

### Exercise

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

$$v = \sqrt{\frac{kq_e^2}{m_e r}}.$$

Substituting  $r_n = a_0 n^2$  we get

$$v_n = \frac{1}{n} \sqrt{\frac{kq_e^2}{m_e a_0}} = \frac{v_1}{n}.$$

The value of  $v_1$  is

$$v_1 = 2.19 \times 10^6 \text{ (m/s)}$$

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

$$F_1 = 8.24 \times 10^{-8} \text{ (N)}$$

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:

$$m_e = 9.1 \times 10^{-31} \text{ (kg)}.$$

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 electron 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

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  $\nu$  as follows:

$$\Delta E = E_m - E_n = h\nu_{nm} \quad m > n.$$

**Exercise 5.1** 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

$$\lambda = \frac{ch}{E_1} \frac{n^2 m^2}{m^2 - n^2} = 91.127(nm) \times \frac{n^2 m^2}{m^2 - n^2}. \quad (5.1)$$

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 (5.1), 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 5.2** According to the the formula (5.1), 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*.

### 5.1.2 Spontaneous Emission and Cavity QED

According to Schrodinger equation, an hydrogen atom with electron in any stationary 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 exciting fields of *Cavity Quantum Electrodynamics* or *cavity QED*.

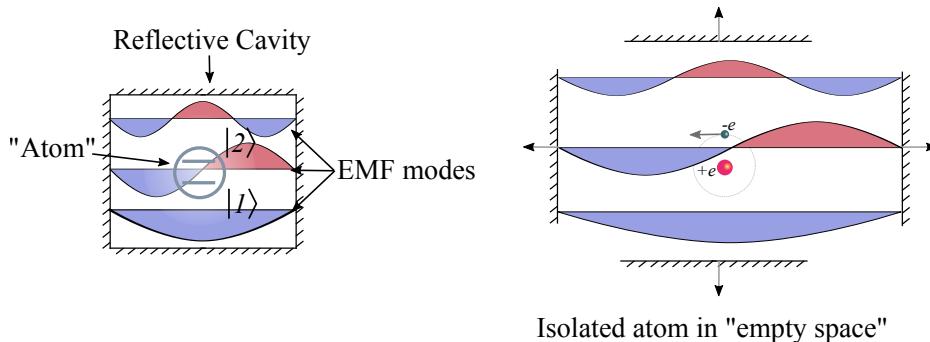


Figure 5.3: Atom in “empty space” is a quantum system in a very large cavity, coupled to the modes-oscillators of electromagnetic field.

## 5.2 Quantum Dots

### 5.3 Photoeffect

### 5.4 Conductors

### 5.5 Maser and Lasers

### 5.6 Entanglement

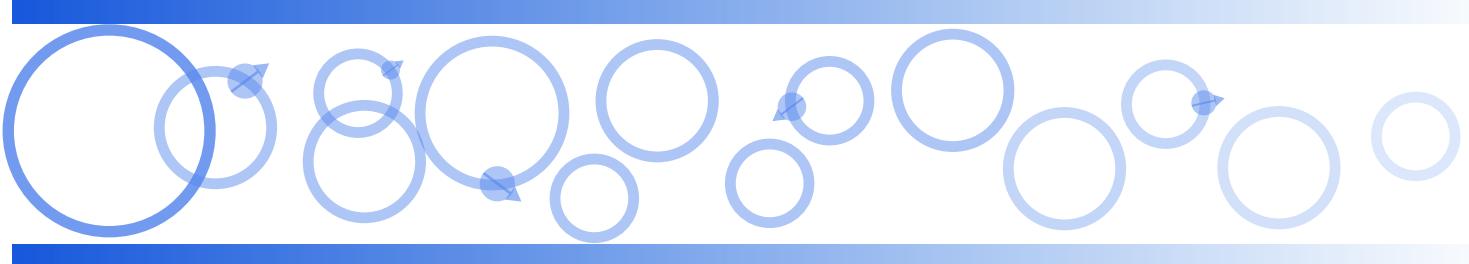
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# Appendix

|          |                             |           |
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## 6. Appendices

### 6.1 Game of Scalars

*Scalar* is a synonym for a *numeric value*, a number. Scalars are the simplest mathematical objects. They are at the bottom of hierarchy of mathematical objects, with *vectors* and *tensors* belonging to the next two levels. In this section we will focus on *function* that operate with numbers.

We will understand *function* as a method of calculating a *unique* output value (*result*) from an input value (*argument*). Symbolic notation:

$$f x = y .$$

This notation agrees with standard way of writing

$$\sin \phi \quad \ln y \quad \text{id } x .$$

Here we mention the most basic mathematical function – *identity function* with simple action:

$$\text{id } x = x .$$

Despite its simple look, the identity function is as important as 0 for addition and 1 for multiplication.

We will surround the argument in parentheses only to avoid confusion when the argument has structure. For example,

$$\sin(\pi + 3) = -\sin 3 \quad \text{but} \quad \sin \pi + 3 = (\sin \pi) + 3 = 3 .$$

#### Function Representation

The idea of function is abstract. Actual computation of the results is concrete and is achieve by a specific method. In other words, every function must be *represented* in some usable form.

The typical ways of representing functions are

- *Symbolic*:  $f x = \sin [3 * (\ln x)^2]$ .
- *Tabular* – output values  $y_i$  for each value of input  $x_i$ .
- *Graphical* – plot a curve in given axes.
- *Schematic* as a box with inputs and outputs (see Figure 6.1).

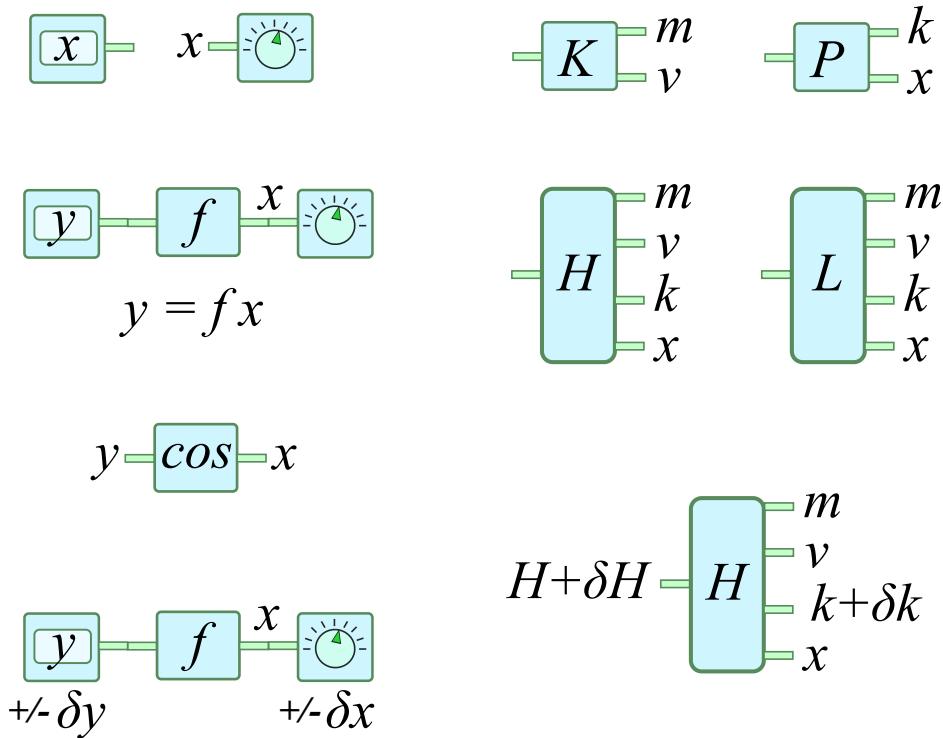


Figure 6.1: Function as a box with input-output.

## Composition

One of the most fundamental concepts in mathematics of functions is their *composition*: Applying functions sequentially. Examples:

$$f \phi = \sin(\cos \phi).$$

The function  $f$  is called *composition* of sin and cos and is denoted as follows:

$$f = \sin \circ \cos .$$

In this expression we wrote the function in *argument-free form* where we dropped the argument  $\phi$  writing the structure of the function  $f$  in terms of other functions.

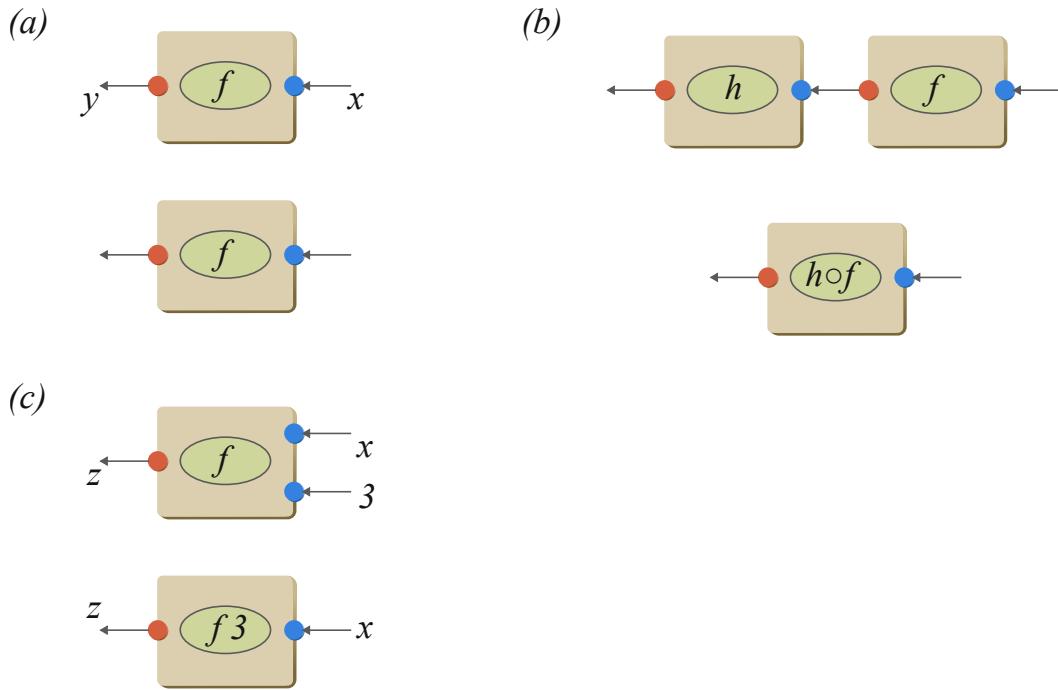


Figure 6.2: (a) Function as a box with input-output. (b) Composing two functions. (c) Partially applying a binary function.

## Arity

The number of arguments that function accepts determines its *arity*. The simplest non-trivial functions (functions with more than zero arguments) are called *unary functions*. Functions accepting two arguments are called *binary functions*; three – *ternary*. Functions with  $n$  arguments are called  $n$ -*ary* functions.

We will focus on unary and binary functions.

## Partial Application

When a binary function has one of its inputs “plugged-in” and the second “open”, we have the case of *partial application*. More generally, when a function with  $n$  arguments has some – but no all – of its inputs fixed, the function is called *partially applied*. For example, if

$$f x y = x * y$$

then  $f 2$  denotes the function  $f$  with its first argument fixed ( $x = 2$ ). As the result, we get a unary function  $g = f 2$  that works as follows

$$g y = 2 * y .$$

The function  $g$  simply doubles the value of its argument.

Together with composition, partial application provides a way to “build” new functions.

### Non-commutativity

When composing functions the order is important. For example:

$$\sin(\cos x) \neq \cos(\sin x)$$

and therefore

$$\sin \circ \cos \neq \cos \circ \sin .$$

The binary operation of composition “ $\circ$ ” is said to be *non-commutative*. The familiar operations addition “ $+$ ” and multiplication “ $*$ ” are *commutative*. Commutativity is useful – it simplifies mathematical reasoning – but not fundamental. Non-commutative operations in mathematics and physics are very important.

### Functions, Functionals, Operators

The idea of function is powerful but somewhat limiting. It is extended to allow acting of arguments of various types.

The usual numerical *function* maps numbers into numbers:

$$f : \text{number} \longrightarrow \text{number} .$$

*Functional* is a kind of *function of function* that maps a given function into numbers:

$$\mathcal{F} : \text{function} \longrightarrow \text{number} .$$

For example, given a function  $f$  functional may return the value of the function in a given point (say  $x = 0$ ):

$$\mathcal{F} f = f 0 .$$

Another example:

$$\mathcal{F} f = \max_{[0, 1]} f$$

returns the maximum value of the argument-function  $f$  in the interval  $[0, 1]$ . One more:

$$\mathcal{F} f = \sum_{i=1}^{i=N} f(i)$$

returns the sum of values of  $f$  on a discrete set of points  $x = i$ . More sophisticated forms of such sums are possible:

$$\mathcal{F} f = \sum_{x_1=a}^{x_n=b} f(x_i) \Delta x_i .$$

The most important functional we will encounter in classical mechanics is the functional of *action*.

Finally, *operators* are functions that act on functions to return a new function:

$$\hat{f} : \text{function} \longrightarrow \text{function} .$$

The tradition is to put a “hat” on top of an operator. Some example of operators:

$$\hat{h} f = h \text{ where } h x = f(2 * x) .$$

$$\hat{g} f = g \text{ where } g x = (f x) + (f [x + 1]) .$$

$$\hat{s} f = s \text{ where } s x = f(f x) .$$

Although these examples are of no immediate use to us, they demonstrate that the idea of a function as the methods of calculating result from an input is a very flexible one.

Once we learn the basics of *kalkulus*, we will encounter the important operator  $\partial$ . Additionally, we will extend the idea of operators to include functions that map *vectors into vectors*.

### Operator Composition

When a function is applied sequentially many times, we may write

$$f(f(f(f x))) .$$

Alternatively, this can be written using the composition operator “ $\circ$ ”:

$$(f \circ f \circ f \circ f) x .$$

Similar expression can be written for an operator:

$$(\hat{g} \circ \hat{g} \circ \hat{g} \circ \hat{g}) f .$$

However, special notation is used for operators that are sequenced like that:

$$\hat{g} \circ \hat{g} \circ \hat{g} \circ \hat{g} = \hat{g}^4.$$

This notation resembles the rule for multiplication:

$$x * x * x * x = x^4.$$

### Multiplexing and Tensor Product

Sometimes it is useful to *join* two mathematical objects (numbers, functions, operators) together without loosing each component. This type of “bundling” or pairing proves very useful in physics for describing systems that consist of several components. A special notation is used to denote operation of this sort:

$$x \otimes y.$$

## 6.2 Kalkulus 101

We will need several basic ideas from the mathematics of infinitely small quantities.

Suppose we study position of a body as function of time. We measure the position at time  $t_1$  and then later at time  $t_2$ . In general, time interval between these measurements can be large (on the scale used for the problem):

$$\Delta t = t_2 - t_1.$$

For example, we can measure position of a planet several months apart. If the time interval is small, we use different notation:

$$\delta t = t_2 - t_1.$$

In the example above, this corresponds to measuring the position of the planet several seconds apart.

For a continuous motion of the planet, we expect small changes in position during small time interval

$$\delta t \quad \rightarrow \quad \delta x, \quad a\delta t \quad \rightarrow \quad a\delta x$$

and, in general:

$$\Delta t \quad \rightarrow \quad \Delta x, \quad a\Delta t \quad \not\rightarrow \quad a\Delta x.$$

We can now speak of *rate of change of position with respect to time*:

$$R = \frac{\delta x}{\delta t}, \text{ and with special notation } \partial_t x = \frac{\delta x}{\delta t}.$$

For example, given the kinetic energy  $K(v) = mv^2/4$  we can find

$$\partial_v K = \frac{\delta K}{\delta v} = \frac{K(v + \delta v) - K(v)}{\delta v}.$$

$$\partial_v K = mv + \frac{m\delta v}{2}.$$

Physicist can neglect the tiny contribution from the second term with  $\delta v$ , while mathematician consideres the value of the expression *in the limit of*  $\delta v \rightarrow 0$ . In any way, we get

$$\partial_v K = mv = p.$$

### Problem

Calculate  $\partial_m K$ .

### Problem

Calculate  $\partial_v \Pi$ .

#### 6.2.1 Taylor Series

Almost all *useful* curves posses the following property: Any piece of a curve can be viewed approximately as a *polynomial curve*, such as a piece of straight line, a piece of parabola, a piece of cubic or higher order polynomial. This is illustrated in the Figure 6.3.

### 6.3 Bernoulli Sum Notation

$\int$  summation sign used by Jacob Bernoulli in *Summae Potestatum*:

$$\int n = 1 + 2 + \dots + n = \frac{1}{2}nn + \frac{1}{2}n, \quad (6.1)$$

$$\int nn = 1^2 + 2^2 + \dots + n^2 = \frac{1}{3}n^3 + \frac{1}{2}nn + \frac{1}{6}n. \quad (6.2)$$

We will use this sign to denote a sum of very large number of very small quantities:

$$\int \delta x = \delta x + \delta x + \dots + \delta x \text{ or } \int \delta x = \delta x_1 + \delta x_2 + \dots + \delta x_n.$$

$$f(x) = a_0 + a_1x + a_2x^2 + \dots + a_nx^n + \dots$$

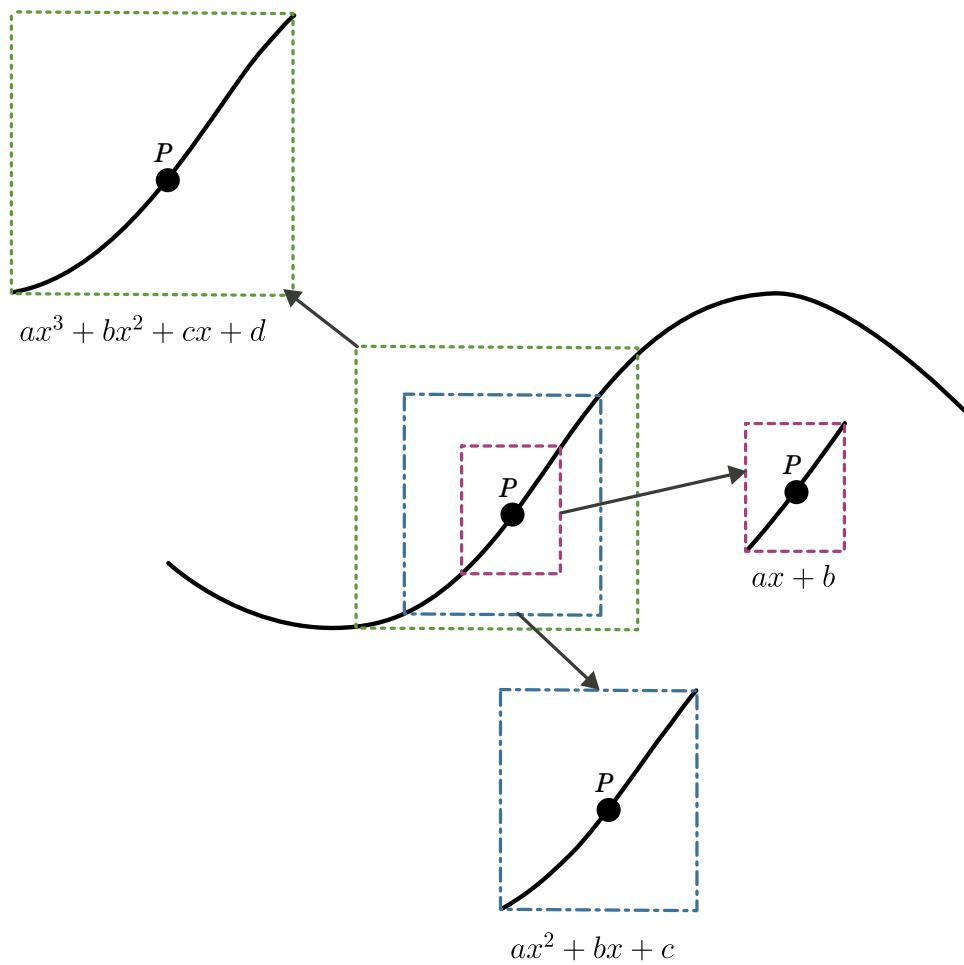


Figure 6.3: Any piece of a sufficiently smooth curve can be approximated with polynomials. The higher degree of polynomial allows higher accuracy of approximation.

NOTE: This is *not an integral*. Integrals have a specific and rigorous mathematical definitions.

## 6.4 Game of Arrows

Arrows or directed line segments provide the simplest model for *vectors*. Vectors are often described as *quantities with magnitude and direction*. This is a useful starting point. We will focus on arrows in a plane.

An arrow has a tail and the head (tip). An arrow can start at any point in the plane – its tail is not attached. But once the tail's position is fixed, the tip uniquely specifies another point in the plane.

Many physical quantities have arrow-like nature: Displacement, velocity, acceleration, force, electric field strength, heat flow, and so on.

We can view arrows as *instructions for movement*. An arrow “says”: Go in that direction that far. This viewpoint leads to a simple rule of combining arrows as a sequence of instructions: First go in this direction that far, then go in another direction that far, and so on. Graphically this is represented with arrows arranged tail-to-tip. This is the basic idea behind *arrow addition*.

### 6.4.1 Operations on arrows

Addition of vectors is a binary vector operation since it takes two vectors as its input and returns the third vector:

$$\text{add } \vec{a} + \vec{b} = \vec{c} .$$

Unary functions on arrows would take a single arrow as input and produce an output:

$$\hat{L} \vec{a} = x \quad \text{or} \quad \hat{M} \vec{a} = \vec{b} .$$

In this example the function  $\hat{L}$  returns a number for every arrow (e.g. the length), and the function  $\hat{M}$  returns another arrow (e.g. copy of the input rotated counter clock-wise by 45 degrees).

Functions on arrows are called *operators* and are written with the “hat” on top of their name.

Since two vectors can differ only in their directions and lengths, the two basic unary operators are scaling

$$\hat{S} \vec{a} = s \vec{a} \quad \text{and rotation} \quad \hat{R}_\theta \vec{a} = \vec{b}$$

where  $\vec{b}$  is rotated relative to  $\vec{a}$  by the angle  $\theta$  in the counter clock-wise direction.

### 6.4.2 Basis. Dimensions. Components

Some arrows can be chosen as “building blocks” for all other arrows. In other words, every arrow in the plane can be written as the combination (linear) of the same two arrows:

$$\vec{a} = a_1 \vec{e}_1 + a_2 \vec{e}_2 \quad \text{and} \quad \vec{b} = b_1 \vec{e}_1 + b_2 \vec{e}_2.$$

The set of arrows  $\vec{e}_1$  and  $\vec{e}_2$  is called *basis*. The coefficients  $(a_1, a_2)$  and  $(b_1, b_2)$  are called *components* of the vectors  $\vec{a}$  and  $\vec{b}$  *relative to the basis*.

The arrows of the basis must point in different directions – they can not be parallel. Such arrows are called *linearly independent*. In the plane the maximum number of linearly independent arrows is 2 (two). Another way to express it is to say that the plane has two *dimensions*. This idea can be applied to “usual” three dimensional space and to more abstract spaces of any number of dimensions.

Using basis and components many useful operations with arrows can be reduced to the algebraic operations with components. The simplest example – addition of two arrows:

$$\vec{c} = \vec{a} + \vec{b} = (a_1 + b_1) \vec{e}_1 + (a_2 + b_2) \vec{e}_2.$$

To find the components of the vector  $\vec{c}$  we simply add components of  $\vec{a}$  and  $\vec{b}$ .

### 6.4.3 Linear Operators. Components

The simplest functions on arrows (*operators*) are the ones that have *linearity*. Using an unary operator as example, linearity conditions are given by

$$\hat{L}(\vec{a} + \vec{b}) = (\hat{L}\vec{a}) + (\hat{L}\vec{b}) \quad \text{and} \quad \hat{L}(x\vec{a}) = x(\hat{L}\vec{a}).$$

Such operator  $\hat{L}$  is called *linear operator*. It is an operator analog of simple algebraic operation of multiplication. Indeed, if  $f x = a * x$ , then

$$f(x + y) = (f x) + (f y) \quad \text{and} \quad f(b * x) = b(f x).$$

Despite its simplicity, linear operators are extremely useful in science.

Due to their linearity, the action of a linear operator on an arbitrary arrow is determined if the action of the operator on the basis arrows is known:

$$\hat{L}\vec{a} = \hat{L}(a_1 \vec{e}_1 + a_2 \vec{e}_2) = [\hat{L}(a_1 \vec{e}_1)] + [\hat{L}(a_2 \vec{e}_2)].$$

Using the linearity again, we get

$$\widehat{L} \vec{a} = a_1[\widehat{L} \vec{e}_1] + a_2[\widehat{L} \vec{e}_2].$$

Now  $\widehat{L} \vec{e}_1$  is just another arrow. Lets denote it  $\vec{f}$ . As any arrow, it can be written in terms of components:

$$\vec{f} = f_1 \vec{e}_1 + f_2 \vec{e}_2.$$

Similarly, denoting  $\widehat{L} \vec{e}_2 = \vec{g}$  we can write

$$\vec{g} = g_1 \vec{e}_1 + g_2 \vec{e}_2.$$

The set of four numbers  $(f_1, f_2, g_1, g_2)$  completely determine how the linear operator  $\widehat{L}$  acts on *any* arrow.

Special notation is used for the components of linear operators. Namely, instead of  $f$  and  $g$  we write

$$\widehat{L} \vec{e}_1 = L_{11} \vec{e}_1 + L_{12} \vec{e}_2,$$

and

$$\widehat{L} \vec{e}_2 = L_{21} \vec{e}_1 + L_{22} \vec{e}_2.$$

The numbers  $L_{ij}$  are called *components of the linear operators* (relative to the chose basis, of course). The choice if indices in  $L_{ij}$  is simple: The first index correponds to the basis arrow being acted on, the second index correponds to the basis arrow in multiplied by. A compact way of writing the action of linear operator is often used:

$$\widehat{L} \vec{e}_i = L_{ij} \vec{e}_j,$$

where the summation over the repeated index  $j$  is implied.

#### 6.4.4 Scalar Product

Two arrows can be compared for their “likeness”, “similarity”, or “degree of alignment”. In other words, two arrows can be compared using a binary operator that results in a number that measures how much two vectors “overlap”:

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

The traditional way to do this is to calculate the area of the rectangle build from  $\vec{a}$  and the *projection* of  $\vec{b}$  onto the direction of  $\vec{a}$ :

$$\hat{\sigma} \vec{a} \vec{b} = ab \cos \theta,$$

where  $\theta$  is the angle between the arrows. *Note:* the same area is obtained from  $\vec{b}$  and the projection of  $\vec{a}$  onto  $\vec{b}$ . The last formula defines *scalar product* (numeric product) of two vectors.

It is important to recognize that scalar product is essentially a binary operator which is also *linear* for each argument – it is *bilinear operator*:

$$\hat{\sigma} \vec{a} (x \vec{b} + y \vec{c}) = x(\hat{\sigma} \vec{a} \vec{b}) + y(\hat{\sigma} \vec{a} \vec{c}).$$

Two arrows that point in perpendicular directions are considered to have zero “alignment”, they are called *orthogonal*.

#### 6.4.5 Conjugate Vectors

Scalar product of two arrows is a binary operator that return a number for each pair of arrows. A simpler case would be an unary linear operator that returns a number for each input arrows. Such operator is easy to construct using scalar product and *partial application*.

Consider a linear operator

$$\hat{L}_a = \hat{\sigma} \vec{a}.$$

By construction it is an unary linear operator that returns a number:

$$\hat{L}_a \vec{b} = \hat{\sigma} \vec{a} \vec{b} = ab \cos \theta.$$

Such unary linear operator can be constructed for every arrow  $\vec{a}$ . In other words, every arrow-vector has a “relative”-operator, called *conjugate vector*. Conjugate vectors are especially useful in the mathematical framework of quantum physics.

### 6.4.6 Quantum Notation

Paul Dirac introduced a powerful notation for vectors in quantum physics. Instead of arrows over letters, a vector is specified by placing the letter between a pair of symbols:

$$\vec{a} \longrightarrow |a\rangle .$$

With this notation we can write all the usual expressions

$$|a\rangle + |b\rangle = |c\rangle \quad \hat{\sigma}|a\rangle |b\rangle = ab \cos \theta .$$

In Dirac notation the conjugate vectors are denoted by “flipping”/ “mirroring” the brackets:

$$\hat{L}_a = \langle a| .$$

The action of this operator on another arrow-vector is beautifully written as follows:

$$\hat{L}_a \vec{b} = \langle a || b \rangle = \langle a | b \rangle .$$

In the last expression the second vertical line is dropped to make the expression neater. The arrow-vectors like  $|b\rangle$  are called *ket*-vectors, the unary linear operators like  $\langle a|$  are called *bra*-vectors. Their scalar-product combination

$$\langle a | b \rangle = ab \cos \theta$$

is called scalar *bracket*.

### 6.4.7 Tensor Product

Scalar product is the simplest type of product of two vectors. Scalar product “downgrades” the result in the following sense: It takes two arrows (vectors) and returns a number, which is one “level” below arrows (vectors) in the hierarchy of mathematical objects. It is impossible to recover the input vectors from the value of their scalar product.

*Tensor product* of two vectors is another type of linear operation with a pair of vectors. The result is a mathematical object one “level” above in the hierarchy of mathematical object – *tensor*. We will not explore more rigorous defintion of tensors.

In essense, tensor product of two vectors “bundles” them up into a new structure, preserving information

about each vector. Symbolically this is denoted as

$$|a\rangle \otimes |b\rangle .$$

Here we used quantum notation for vectors and the conventional symbol “ $\otimes$ ” for tensor product.

Tensor product is a versatile tool. It can also be applied to *operators*! Suppose we have operators  $\hat{J}$  and  $\hat{L}$ , then we can “bundle” them into a more complex structure:

$$\hat{J} \otimes \hat{L} .$$

Such structures are often used when we need to act on tensor product of vectors:

$$(\hat{J} \otimes \hat{L}) (|a\rangle \otimes |b\rangle) .$$

Despite its complicated look, the interpretation of this expression is simple:

$$(\hat{J} \otimes \hat{L}) (|a\rangle \otimes |b\rangle) = (\hat{J}|a\rangle) \otimes (\hat{L}|b\rangle) .$$

In other words, tensor product of operators act on tensor product of arrows/vectors “in parallel”: The first operator acts on the first arrow, the second operator acts on the second arrow, preserving the tensor product structure.

Tensor product is used to “bundle” several vectors that correspond to different parts of a multi-part system (atoms with many electrons, cavities with many photons, and similar).

Often more condensed form of tensor product is used. For example:

$$|a\rangle \otimes |b\rangle \otimes |c\rangle \otimes |d\rangle = |a\rangle |b\rangle |c\rangle |d\rangle .$$

#### 6.4.8 Projectors

*Projectors* are special operators built using tensor product of bra and ket vectors (arrow and its conjugate):

$$\hat{P} = |a\rangle \otimes \langle a| .$$

The tensor product symbol is often omitted and projector is written as follows:

$$\hat{P} = |a\rangle \langle a| .$$

Projector acts on an arbitrary arrow-vector  $|b\rangle$  in a simple way:

$$\hat{P}|b\rangle = |a\rangle\langle a||b\rangle = |a\rangle\langle a|b\rangle = (ab \cos \theta)|a\rangle.$$

Thus, the result is a vector parallel to  $|a\rangle$  and the action of the projector consists in *projecting*  $|b\rangle$  onto  $|a\rangle$ .

#### 6.4.9 Vector Space. Hilbert Space

All possible vectors taken together form a special set called *vector space*. Vector space is more than a set because of all interesting and useful operations that exist for vectors.

Vector spaces may have different number of dimensions. We only focused on arrow in a plane. Plane has two basis arrows and is therefore two dimensional. The familiar space around us is three dimensional. Vector space can be 100-dimensional, and all ideas (components) and operations (addition, scalar product) would work similarly to 2 and 3 dimensions.

In quantum physics vectors space with infinite number of basis vectors are needed. Such spaces (with some additional mathematical requirements which are of no special importance) are called *Hilbert spaces*.

The infinite number of components for vectors should not scare us. Many mathematical functions can be viewed as vectors with infinite number of components. And mathematical functions useful for physical description of particles form Hilbert space.

## 6.5 Compound Numbers

The machinery of arrow-vectors and operators on them allows us to see connection between arrow-vectors in a plane and *complex numbers*. Since we will not introduce and discuss complex numbers in a conventional way, we will use unconventional name for them – *compound numbers*.

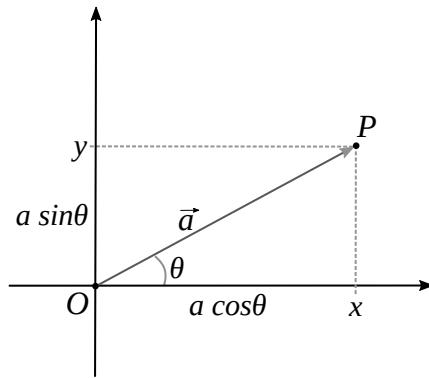


Figure 6.4: A point in a plane can be specified by an arrow-vector, or using a pair of numbers – Cartesian coordinates of the point.

A point in a plane is uniquely specified by a pair of Cartesian coordinates  $(x, y)$ . Alternatively, the point can be specified by the arrow-vector connecting the point and the origin of the coordinates, as shown in the Figure

6.4. If we choose the basis vectors  $\vec{e}_1$  and  $\vec{e}_2$  along the coordinate axes, then we can write

$$\vec{a} = x \vec{e}_1 + y \vec{e}_2. \quad (6.3)$$

Thus, there exists a natural connection between planar arrow-vectors and pairs of numbers  $(x, y)$ .

Any vector  $\vec{a}$  can be obtained from the basis vector  $\vec{e}_1$  by appropriate scaling and rotation:

$$\vec{a} = a \hat{R}(\theta) \vec{e}_1$$

In particular, the second basis vector is given by:

$$\vec{e}_2 = \hat{R}(\pi/2) \vec{e}_1 = \hat{J} \vec{e}_1,$$

where we introduced a special symbol  $\hat{J}$  for a 90-degree rotation. The operator  $\hat{J}$  has an interesting property: Applied twice to any vector, it flips the direction of the latter:

$$\hat{J}(\hat{J} \vec{a}) = (\hat{J} \circ \hat{J}) \vec{a} = -\vec{a}.$$

Symbolically this can also be written in the argument-free form:

$$\hat{J}^2 = -\hat{I} = -1.$$

Using the operator  $\hat{J}$ , we can rewrite the expression (6.3) as follows:

$$\vec{a} = (x + y \hat{J}) \vec{e}_1.$$

Given that  $x = a \cos \theta$ , and  $y = a \sin \theta$ , we obtain

$$\vec{a} = a(\cos \theta + \sin \theta \hat{J}) \vec{e}_1,$$

from which follows the expression for the rotation operator

$$\hat{R}(\theta) = \cos \theta \hat{I} + \sin \theta \hat{J}. \quad (6.4)$$

Rotation of a vector by an angle  $\theta$  can be performed as a single step, or as a sequence of  $N$  rotations, each by

a smaller step  $\delta\theta = \theta/N$ :

$$\hat{R}(\theta) = \hat{R}(\delta\theta) \circ \hat{R}(\delta\theta) \circ \dots \circ \hat{R}(\delta\theta) = [\hat{R}(\delta\theta)]^N.$$

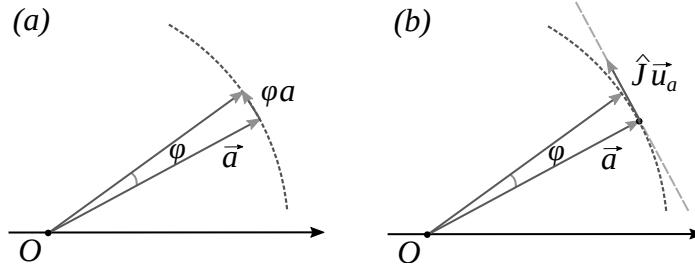


Figure 6.5: Rotation of a vector  $\vec{a}$  by a tiny angle  $\phi$ .

When a vector  $\vec{a}$  is rotated by a tiny angle  $\phi$ , its tip travels along the arc of the length  $a\phi$ , in the direction perpendicular to the vector itself, see Figure 6.5. The unit length vector, pointing perpendicular to  $\vec{a}$  can be obtained from a unit vector  $\vec{u}_a$  pointing along  $\vec{a}$ :

$$\hat{J}\vec{u}_a = \hat{J}\left(\frac{\vec{a}}{a}\right).$$

As the result of the rotation by a tiny angle  $\phi$ , the vector  $\vec{a}$  becomes

$$\hat{R}(\phi)\vec{a} = \vec{a} + a\phi(\hat{J}\vec{u}_a) = \vec{a} + \phi\hat{J}\vec{a} = (1 + \phi\hat{J})\vec{a}.$$

Applying this to the relation

$$\hat{R}(\theta) = [\hat{R}(\delta\theta)]^N$$

we arrive at

$$\hat{R}(\theta) = [(1 + \delta\theta\hat{J})]^N = [(1 + \frac{\theta\hat{J}}{N})]^N.$$

In the limit of ever-smaller steps ( $N \rightarrow \infty$  and  $\delta\theta \rightarrow 0$ ), the result becomes the famous limit

$$\lim_{N \rightarrow \infty} \left(1 + \frac{x}{N}\right)^N = e^x.$$

We thus discover the following expression for the rotation operator  $\hat{R}(\theta)$ :

$$\hat{R}(\theta) = e^{\theta\hat{J}},$$

Comparing this with the expression (6.4), we find the important relation between two different representations of the rotation operator  $\hat{R}(\theta)$ :

$$e^{\theta \hat{J}} = \cos \theta + \hat{J} \sin \theta.$$

So far we have established connections between different ways to represent points in a plane:

- (a) coordinate pair  $(x, y)$ ,
- (b) arrow-vector  $\vec{a}$ ,
- (c) operator sum  $z(x, y) = x + y\hat{J}$ ,
- (d) operator product  $z(a, \theta) = ae^{\theta \hat{J}}$ .

Neither of these representations is exceptionally advantagous. Different problems may benefit from using different approaches.

We will call the representations  $z = x + y\hat{J}$  and  $z = ae^{\theta \hat{J}}$  *composite numbers*. Composite numbers provide another approach to problems that involve points in a plane. Anything that can be analyzed and solved using either Cartesian coordinates  $(x, y)$  or arrow-vectors  $\vec{a}$  can also be treated using composite numbers.

Which form of composite numbers works best: sum  $z = x + \hat{J}y$  or product  $z = ae^{\theta \hat{J}}$ ? The answer depends on the type of operation we want to perform. Given a pair of composite numbers

$$z_a = x_a + y_a \hat{J} = ae^{\theta_a \hat{J}},$$

and

$$z_b = x_b + y_b \hat{J} = be^{\theta_b \hat{J}},$$

findind their sum  $z_c = z_a + z_b$  is easier using sum-form:

$$z_c = (x_a + x_b) + (y_a + y_b) \hat{J},$$

while the product of two composite numbers  $z_c = z_a z_b$  is calculated easier using their product form:

$$z_c = abe^{\theta_a \hat{J}} e^{\theta_b \hat{J}}.$$

The last expression can be simplified if we use the trigonometric identity

$$\cos \theta \cos \phi - \sin \theta \sin \phi = \cos(\theta + \phi)$$

and the property  $\widehat{J} \circ \widehat{J} = -1$ :

$$z_c = ab(\cos \theta_a + \sin \theta_a \widehat{J})(\cos \theta_a + \sin \theta_a \widehat{J}) = ab[\cos(\theta_a + \theta_b) + \sin(\theta_a + \theta_b)\widehat{J}] .$$

We deduce that

$$z_c = abe^{\theta_a \widehat{J}} e^{\theta_b \widehat{J}} = abe^{(\theta_a + \theta_b)\widehat{J}} .$$

Since a composite number can be represented by a combination of scaling and rotation, the interpretation of the product of two composite numbers is clear: To multiply a number  $z_a$  by a number  $z_b$ , we must scale the arrow-vector  $\vec{a}$  by a factor  $b$  – the length of the arrow-vector  $\vec{b}$  – and rotate it by an angle  $\theta_b$ .

Finally, it is evident that multiplication of composite numbers is commutative:

$$z_c = z_a z_b = z_b z_a .$$

### Composition Rule

The property

$$z_c = z_a z_b = abe^{(\theta_a + \theta_b)\widehat{J}}$$

can be anticipated from the operator form for the composite numbers. Indeed, we could write

$$z_c = z_a z_b = ab\widehat{R}(\theta_a)\widehat{R}(\theta_b)$$

and notice that a sequence of two rotations can be replaced with a single rotation by the combined angle:

$$z_c = ab\widehat{R}(\theta_a + \theta_b) = abe^{(\theta_a + \theta_b)\widehat{J}} .$$

## 6.6 Probability

The concept of probability has two basic definitions. The first definition involves *relative frequency*  $f$ :

$$f_{result} = \frac{N_{result}}{N_{tries}} .$$

To understand this formula, consider a simple experiment of throwing a 6-sided die many times ( $N_{tries} \gg 1$ ). Suppose we are interested in how many times the face value is divisible by 3, denoting the number of times as  $N_{result}$ . The more times we throw, the more times we will see values 3 and 6 (the only numbers of the die

that we multiples of 3), but the ratio of  $N_{result}/N_{tries}$  will be approaching and fluctuating around some number  $f_{result}$ . The Figure 6.6 illustrates this situation using real die and a “simulated” die using computer-generated pseudo-random numbers.

## 6.7 Math Goodies

### 6.7.1 Key Functions

#### Power Function

$$x^n, \quad \partial_x x^n = nx^{n-1}.$$

#### Trigonometry 101

Basic trigonometric function is

$$trg \theta = \vec{1}_\theta = (x, y).$$

The function  $trg$  maps any number  $z = L$  from a number line into a point on a circle with unit radius, as shown in the Figure 6.9.

The point  $P$  on the circles can be specified using a unit-length vector  $\vec{1}_\theta$  having the angle  $\theta = L$  with the horizontal. If Cartesian coordinates are used, the point  $P$  can be specified by a pair of coordinates  $(x, y)$ . The  $x$  coordinate in this case defines the trigonometric function  $\cos L$ , whereas the  $y$  coordinate defines the trigonometric function  $\sin L$ .

$$\cos \theta, \sin \theta, \quad \partial_x \sin x = \cos x, \quad \partial_x \cos x = -\sin x.$$

#### Exponential Function

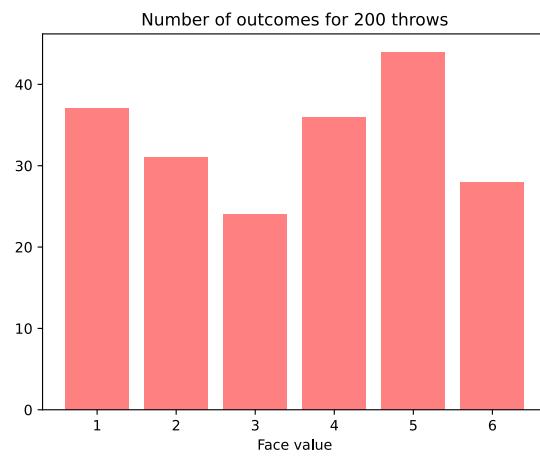
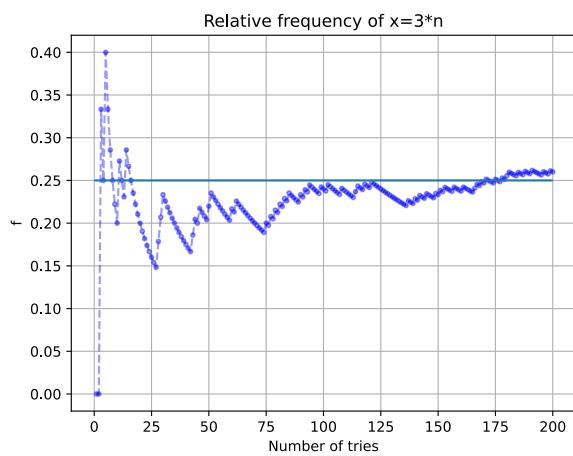
$$e^x, \quad \partial_x e^x = e^x.$$

### 6.7.2 Polynomial Form

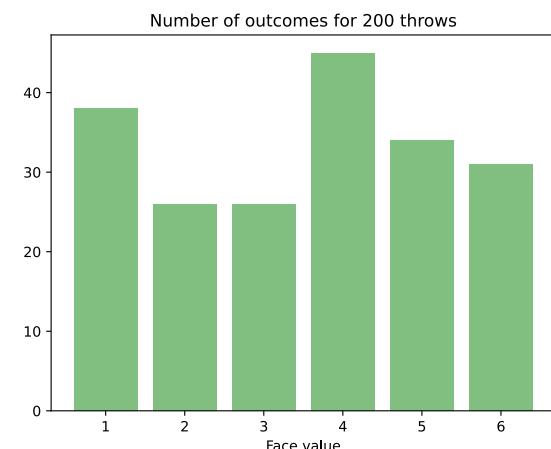
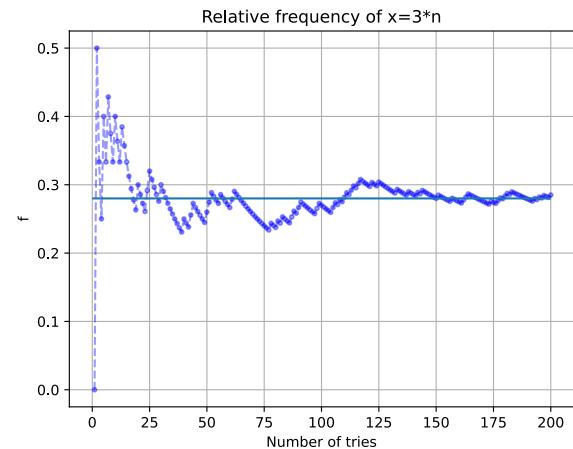
General polynomial of degree  $n$ :

$$P_n(x) = a_0 + a_1 x + a_2 x^2 + \dots a_n x^n.$$

(a)



(b)



(c)

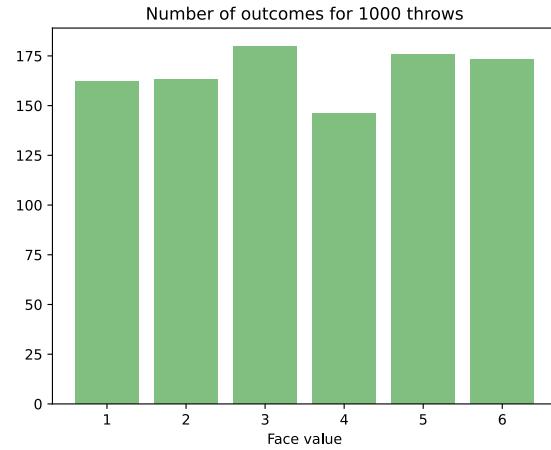
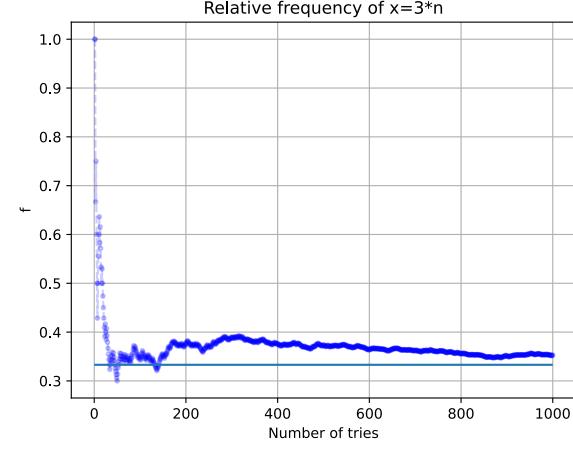


Figure 6.6: Relative frequency and histogram of outcomes for (a) Real die, (b) Pseudo-random number generator (PRNG) for a short sample size, (c) PRNG for a larger sample size.

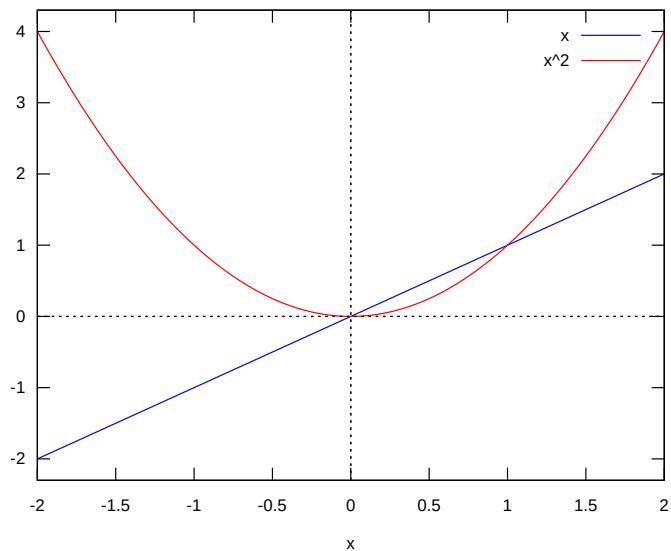


Figure 6.7: Power function  $f(x) = x^n$  for  $n = 1, 2$ .

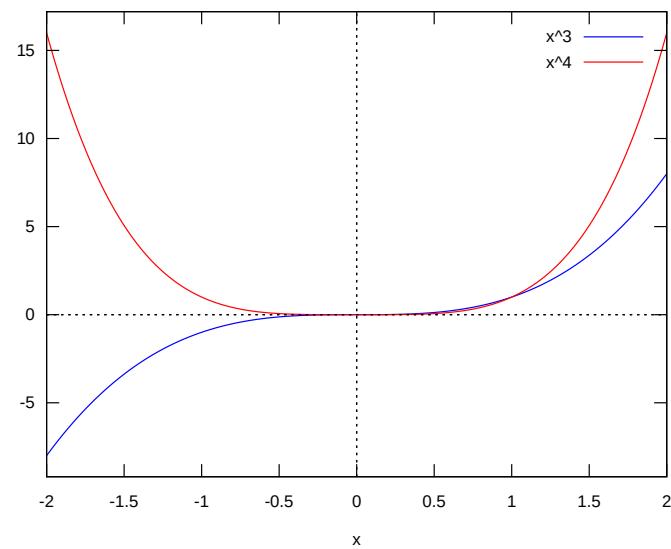


Figure 6.8: Power function  $f(x) = x^n$  for  $n = 3, 4$ .

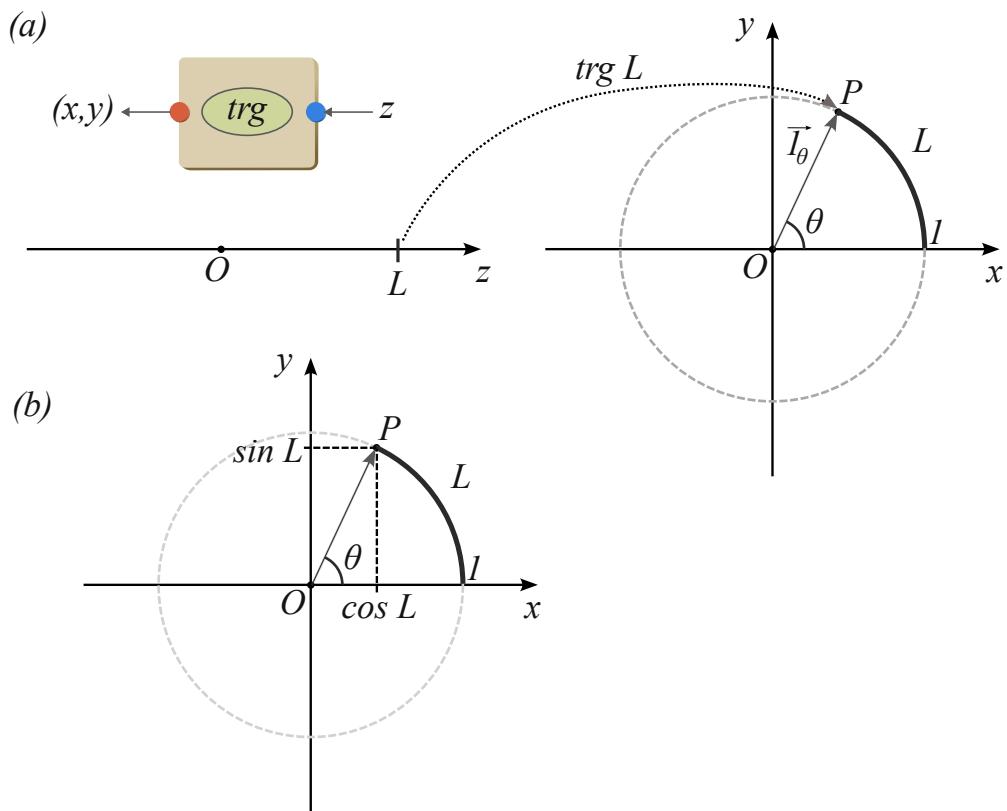
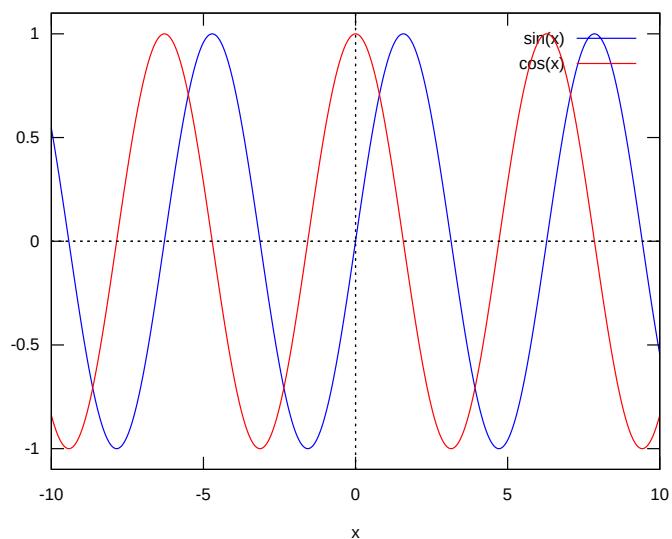


Figure 6.9: (a). (b).

Figure 6.10: Trigonometric functions  $\sin$  and  $\cos$ .

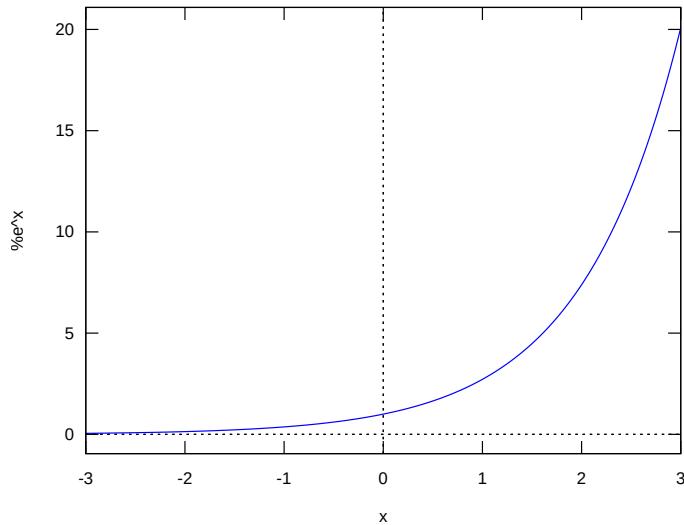


Figure 6.11: Exponential function  $e^x$ .

### Power

$$(1+x)^n \approx 1 + nx + \frac{n(n-1)x^2}{2}$$

### Trigonometric

$$\cos \theta \approx 1 - \frac{\theta^2}{2}, \quad \sin \theta \approx x - \frac{\theta^3}{6}.$$

### Exponential

$$e^x \approx 1 + x + \frac{x^2}{2} + \frac{x^3}{6} + \dots + \frac{x^n}{n!}.$$

### 6.7.3 Approximations

#### Power function

$$(1+x)^n \approx 1 + nx \quad \text{for } x \ll 1.$$

First observe that

$$(1+x)^0 = 1 + 0 \cdot x,$$

$$(1+x)^1 = 1 + 1 \cdot x,$$

$$(1+x)^2 = 1 + 2 \cdot x + x^2,$$

$$(1+x)^3 = 1 + 3 \cdot x + 3x^2 + x^3.$$

If it is true that

$$(1+x)^n = 1 + n \cdot x + r,$$

where  $r$  is the remainder of expression at most  $nx^2$ , then we can write

$$(1+x)^{n+1} = (1+x)(1+x)^n = (1+x) + n(1+x)x + r(1+x) = 1 + (n+1)x + r',$$

where  $r'$  is the remainder of expression at most  $nx^2$ .

## 6.8 Ancient Mechanics

Archaic mechanics – Aristotle. Ancient Mechanics – Galilei-Newton. The goals are: *describe, explain, predict* motion. Basic concepts are position, velocity, acceleration, jerk:

$$x, \quad v = \partial_t x, \quad a = \partial_t v, \quad b = \partial_t a.$$

These are *kinematical* quantities.

Mechanics also studies *dynamical* quantities, such as mass, momentum, force, energy:  $m, p, F, E$ .

Momentum in Galilei-Newtonian mechanics is

$$p = mv.$$

A modern formula:

$$P = \left( \frac{E_0}{\sqrt{1 - v^2/c^2}}, \frac{E_0 v}{\sqrt{1 - v^2/c^2}} \right) \quad E_0 - \text{energy of a body at rest}.$$

1. Consider a particle at rest at  $x$ . Answer the question: What causes the particle to be at  $x$ ?
2. Consider a particle moving with constant speed  $v$ . Answer the question: What causes the particle to move with constant speed  $v$ ?
3. Consider a particle moving with constant acceleration  $a$ . Answer the question: What causes the particle to move with constant acceleration  $a$ ?

The answer to the last question is given by Newton:

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

More modern way of expressing the same idea is

$\partial_t p = F.$

Forces are measures of *interaction* between objects and are *causes* of changes in momentum.

### Constant Force

When  $F = \text{const}$ , we have

$$\delta p = F \delta t \quad \text{and} \quad p = \int \delta p = F \int \delta t = Ft.$$

From  $p = mv$  and  $a = F/m$  we find for constant force:

$$v = at.$$

Work done by a constant force when moving a body by amount  $\Delta x$  is  $\Delta W = F\Delta x$ . For tiny changes

$$\delta W = F\delta x = Fv\delta t.$$

On the other hand,  $\delta v = F\delta t/m$  and therefore  $\delta t = m\delta v/F$ . Plug in into  $\delta W$  to find

$$\delta W = Fv \frac{m\delta v}{F} = p\delta v.$$

Total work done

$$W = \int \delta W = \int p\delta v.$$

Plotting  $p$  vs  $v$  – see Figure 6.12(a) – shows that the sum gives the area of the triangle, therefore

$$W = \frac{mv^2}{2} = E_k.$$

This is *kinetic energy* of the body – the energy due to motion.

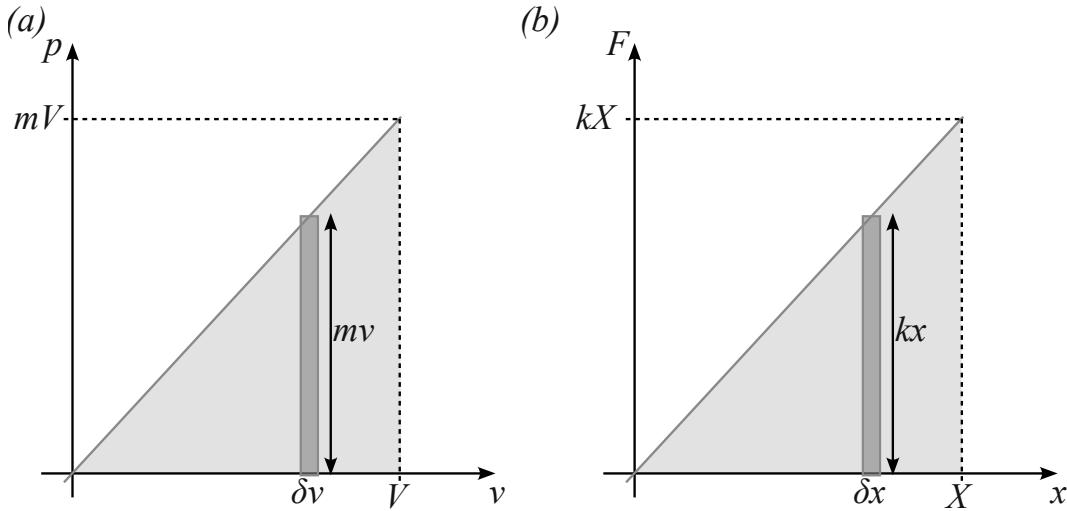


Figure 6.12: (a). (b)

Suppose we apply constant force to a body. If this force balances the force of gravity  $mg$ , then with tiny kick of velocity  $\delta v$  the body will slowly go up. If the vertical distance traveled by the body is  $h$ , then the total work

done by the force  $F$  is

$$W = Fh = mgh = E_p.$$

This is *potential energy* of a body in constant gravitation field.

The sum of kinetic and potential energies of a body is called its *total mechanical energy*:

$$E = E_k + E_p.$$

### Linear Force

An elastic spring with the lengths  $L$  in “relaxed” state can be stretched (compressed) by the amount  $x$  when the force

$$F = kx$$

is applied. The constant  $k$  is called *spring constant* and it quantifies the stiffness/rigidity of the spring.

The total work done by the force applied to the spring is found by summing up tiny steps:

$$W = \int \delta W = \int F \delta x.$$

Plotting  $F$  vs  $x$  it becomes clear, similarly to the calculation of the kinetic energy, that the total work equals to the area of the triangle:

$$W = \frac{kx^2}{2} = E_p.$$

This is the *potential energy* of stretched spring.

### Energy and Force

The definition of work and the relationship between work and potential energy suggest the following relationship between potential energy of an object and force applied to it:

$$F_O = \frac{\delta W}{\delta x} = \frac{\delta E_p}{\delta x} = \partial_x E_p.$$

This is the force  $F_O$  that needs to be applied to the object *from the outside* (for example, pulling the object against the spring). If we are looking for forces *inside the system* (for example, the force from the spring to the object),

then we need to change the direction by adding the negative sign:

$$F = -\partial_x E_p .$$

### Problem

The potential energy of gravitational interaction between masses  $m$  and  $M$  is

$$E_p = -G \frac{Mm}{r} .$$

Using the notation  $r = x$  and the relationship between force and energy, find the force between the massive objects.

#### 6.8.1 Circular Motion

When a body is moving with constant speed  $v$  in a circle of radius  $r$  it makes one full revolution in time (called *period of revolution*):

$$T = \frac{2\pi r}{v} .$$

Using the concept of angular speed  $\omega = 2\pi/T$  we find

$$v = \omega r .$$

The direction of velocity  $\vec{v}$  is always perpendicular to the radius-vector  $\vec{r}$ :

$$\vec{v} = \omega r (\hat{J} \vec{u}_r) = (\omega r) (\hat{J} \frac{\vec{r}}{r}) = \omega \hat{J} \vec{r} .$$

In tiny interval of time  $\delta t$  the tiny changes of position  $\delta \vec{r}$  and velocity  $\delta \vec{v}$  are similarly related:

$$\delta \vec{v} = \omega \hat{J} \delta \vec{r} .$$

Therefore, the acceleration is

$$\vec{a} = \frac{\delta \vec{v}}{\delta t} = \omega \hat{J} \frac{\delta \vec{r}}{\delta t} = \omega \hat{J} \vec{v} .$$

Plugging  $\vec{v} = \omega \hat{J} \vec{r}$  and using the fact  $\hat{J} \circ \hat{J} = -\hat{I}$ , we find

$$\vec{a} = -\omega^2 \vec{r}.$$

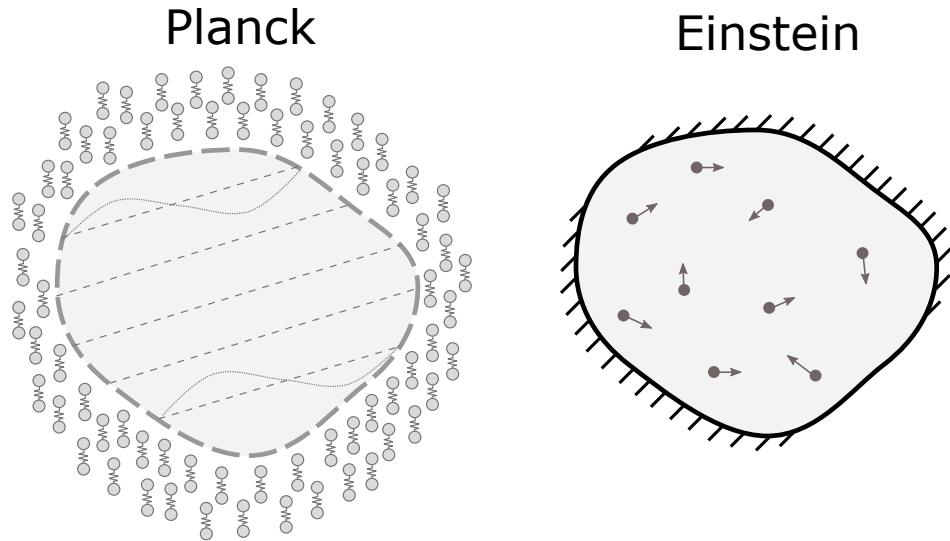
The magnitude of the acceleration for circular motion with constant speed is thus

$$a = \omega^2 r = \frac{v^2}{r^2} r = \frac{v^2}{r}.$$

## 6.9 Physics

### 6.9.1 Black-body Radiation

It is an interesting fact that electromagnetic radiation can (in certain situations) be assigned a definite temperature.



*Figure 6.13: Electromagnetic radiation trapped inside a cavity within any body will reach thermal equilibrium with that body – will have the same temperature. The spectrum – energy vs frequency (or wavelength) – is called black-body spectrum. Max Planck analyzed the spectrum assuming the material of the cavity is made of little oscillators that absorb energy in small portions – quanta of energy. Albert Einstein performed the analysis assuming that the radiation propagates within the cavity as little “parcels” of energy, later called photons.*

### 6.9.2 Spin

#### Electron

Electron is an elementary particle with the following physical characteristics:

- (a) Mass  $m_e$ .
- (b) Electric charge  $q_e$  (monopole, scalar).

(c) Magnetic “charge”  $\mu_e$  (dipole, vector).

Neither of these three can be altered: Electron can not absorb a photon to become more massive; it is impossible to strip a charge from electron to make it neutral; there is no way to “add” magnetic moment to an electron.

### Lorentz Force

### Magnetic Moment

### “Spin” and Spin

### 6.9.3 Writing Notes

It very important to write your notes and solutions clearly. This is a great skill that you should develop in this course. Please examine the following handwritten notes. The first is the page from Albert Einstein's notebook, the second from Erwin Schrodinger's, and the last one is a simple example of how one would write up a solution to a kinematic problem from pre-assessment.

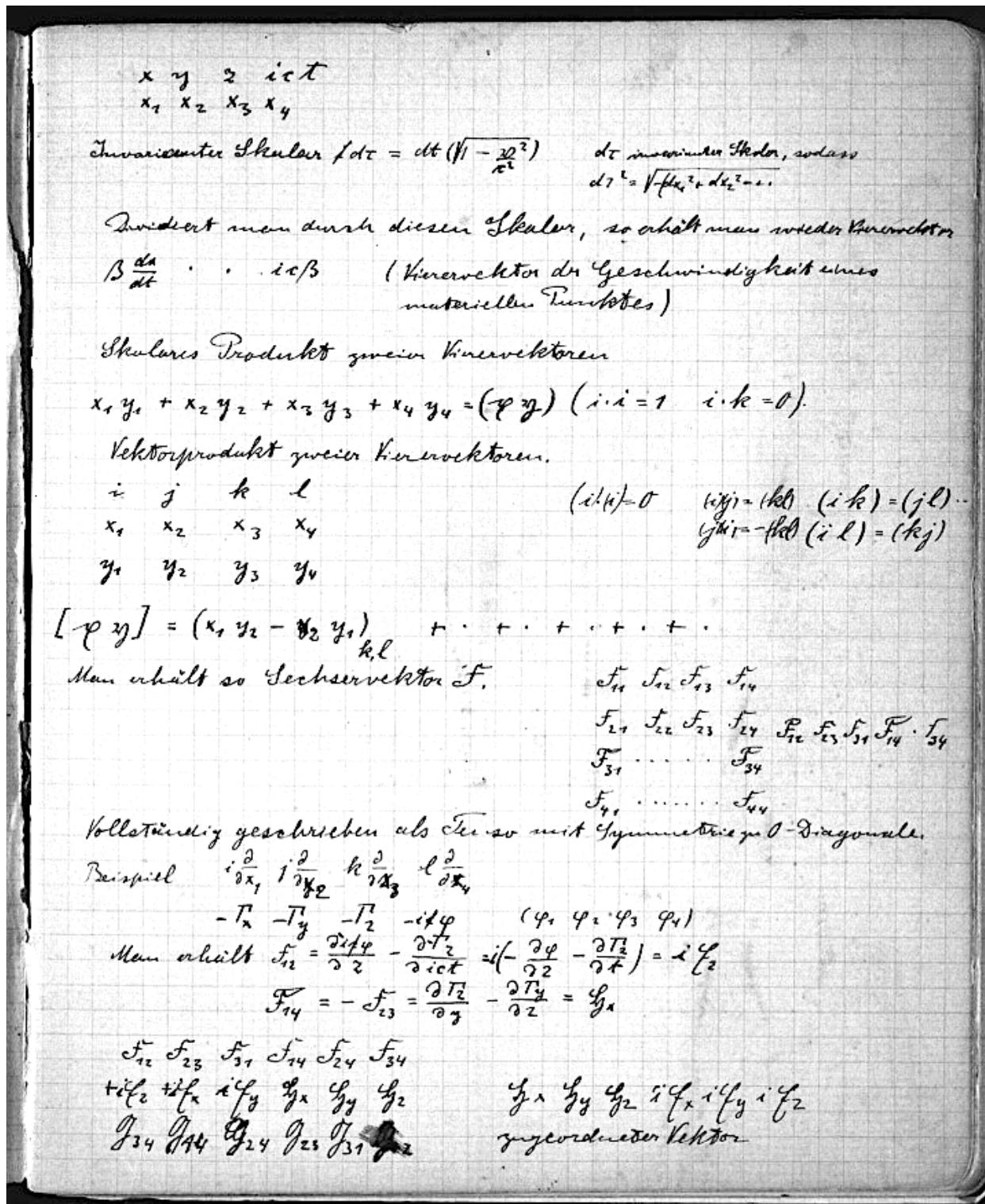


Figure 6.14: Einstein's Notebook from Zurich.

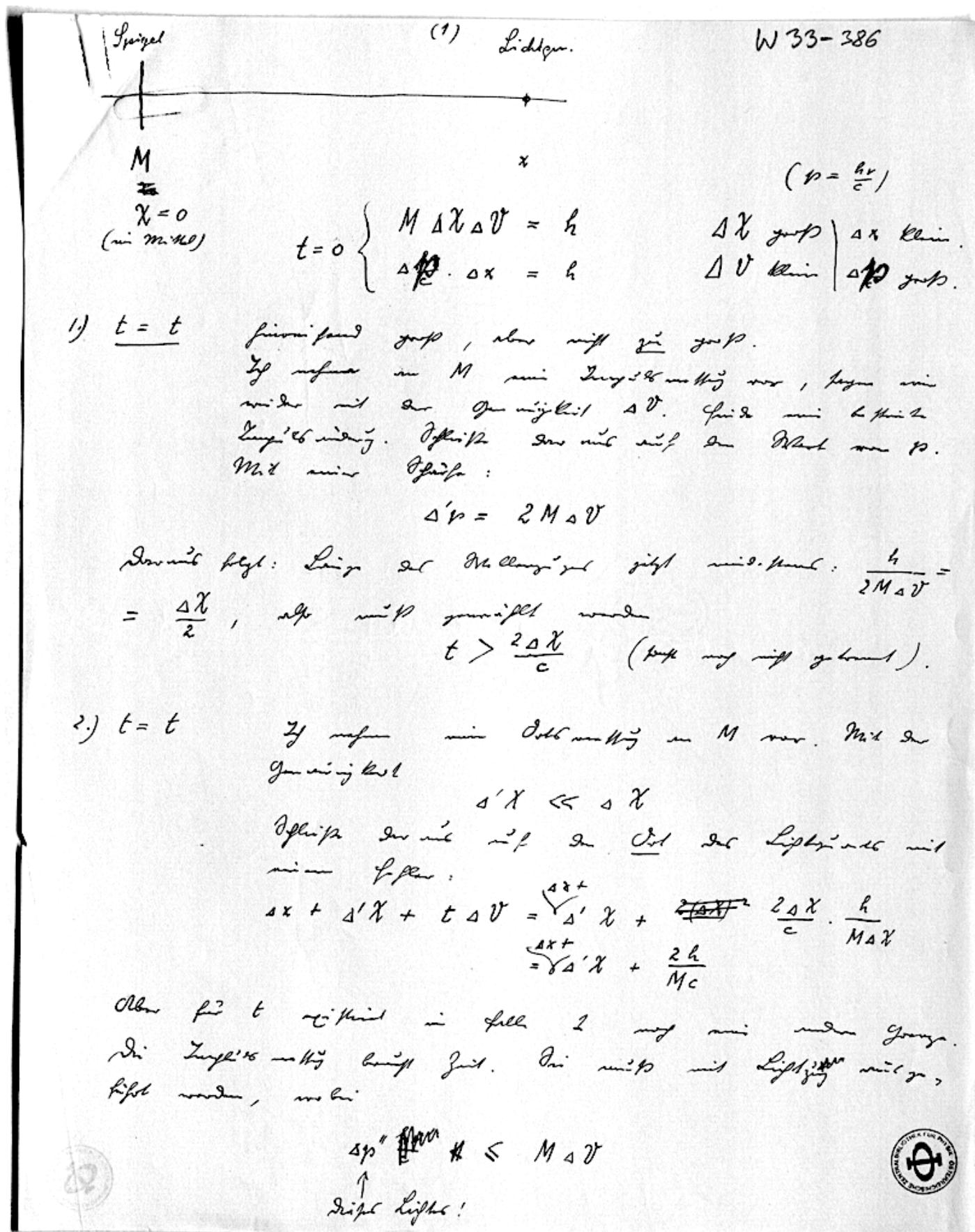
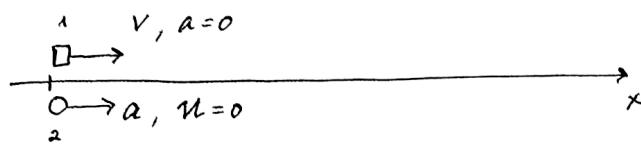


Figure 6.15: Schrodinger's Notebook.

## Problem B3

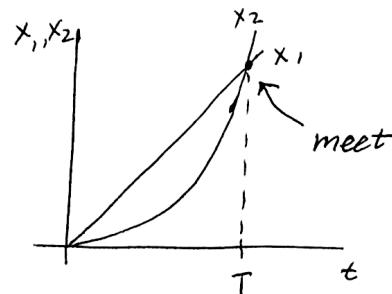


Position of car 1:

$$x_1 = vt$$

car 2:

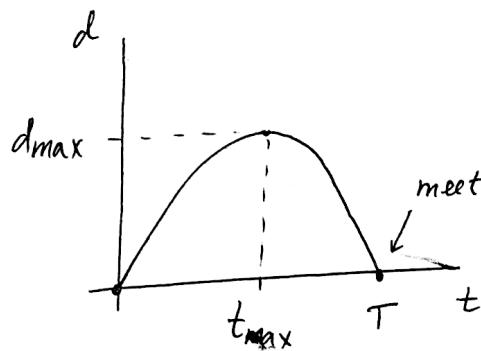
$$x_2 = \frac{at^2}{2}$$



Both meet when distance

$$d = x_1 - x_2 = vt - \frac{at^2}{2} = 0$$

$$d = vt \left(1 - \frac{at}{2v}\right) = 0 \quad \text{at } t=0 \quad t=T = \frac{2v}{a}$$



$$d(t) = vt - \frac{at^2}{2}$$

↑  
parabola, upside down

Maximum at

$$t_{\max} = T/2 = \frac{v}{a}$$

$$d_{\max} = d(t_{\max}) = \frac{v^2}{a} - \frac{v^2}{2a} = \frac{v^2}{2a}$$

For  $v = 5 \text{ m/s}$ ,  $a = 10 \text{ m/s}^2$

$$d_{\max} = \frac{25}{20} = \frac{5}{4} = 1.25 \text{ m}$$

Figure 6.16: Handwritten Solution.

