An Integrated, Quantitative Introduction to the Natural Sciences, Part 1: Dynamical Models[1]

Fall 2011, last updated April 26, 2011

---

[1] Notes from the Integrated Science course for first year undergraduate students at Princeton University. The course is an alternative to the introductory physics and chemistry courses, and is intended to encourage students to think quantitatively about a much broader set of phenomena (including, especially, the phenomena of life) than in the usual introductory examples. We assume that students are comfortable with calculus, and have had some exposure to the ideas and vocabulary of high school physics and chemistry. This module about dynamical models comes (mostly) in the first half of the Fall semester. All inquires can be addressed to `integratedscience@princeton.edu`; current students should refer to `https://blackboard.princeton.edu` for up–to–date course materials.

Preface

As we hope becomes clear, our point of view in this course is rather different from that expressed in conventional introductory science courses. One consequence of this is that we can't simply send you to a standard textbook. These lecture notes, then, are meant to be something that approximates a book, or more precisely a set of books, plus an extra volume for the labs. You'll see that even the first volume of this project is far from finished. We hope that, as with the rest of the course, you'll view this as a collaborative effort between students and faculty, and give us feedback on what is missing from the notes, or on what needs to be improved.

Relation to the lectures

This all needs to be revised

These notes are not an exact record of the lectures, not least because we hope the lectures (and the lecturers) are still alive enough to be evolving from year to year. We do try to cover the same topics, though, in more or less the same order. Because the match to the lectures is loose, we suspect that this text is not a substitute for the notes which you would take during the lectures. On the other hand, knowing that some of the details are written down here means that you don't have to worry quite so much about writing down every word or equation.

For Fall 2010, the rough match between lectures and notes, including some material to be covered primarily in precepts, is as follows:

0. Introduction
  0.1. A physicist's point of view .... F 17 Sep
  0.2. A biologist's point of view .... M 20 Sep
  0.3. A chemist's point of view .... W 22 Sep

1. Newton's laws, chemical kinetics, ...
  1.1 Starting with $F = ma$ .... F 24 Sep

1.2 Chemical reactions: a dynamic perspective .... M 27 Sep
1.3 Radioactive decay and the age of the solar system ..... W 29 Sep
1.4 Using computers to solve differential equations .... (precept)
1.5 Simple circuits and population dynamics .... (precept)
1.6 The complexity of DNA sequences .... F 1 Oct

2. Resonance and response
2.1 The simple harmonic oscillator .... M 4 Oct
2.2 Magic with complex exponentials .... W 6 Oct
2.3 Damping, phases and all that .... F 8 Oct
2.4 Linearization and stability .... M 11 & W 13 Oct
2.5 Stability in a real genetic circuit .... F 15 Oct
2.6 The driven oscillator .... M 18 Oct
2.7 One dimensional waves .... W 20 & F 22 Oct

3. Energy conservation
3.1 Kinetic and potential energies .... M 25 Oct
3.2 Conservative forces and conservation of energy .... W 27 Oct
3.3 Collisions .... F 29 Oct

4. We are not the center of the universe
3.1 Conservation of $\vec{P}$ and $\vec{L}$ .... M 13 Dec
3.2 Universality of gravitation .... Tu 14 Dec
3.3 Kepler's laws .... W 15 Dec
3.6 Biological counterpoint .... Th 16 Dec

The second half of the Fall semester will be covered in a separate volume.

Problems

We cannot possibly overemphasize the importance of derivation as opposed to memorization. Science is *not* a long list of facts, but rather a structure for relating many different observations to one another (more about this soon). Correspondingly, it is not enough for you to learn to recite things that we show you in the lectures; we want you to develop the skills to derive things for yourself, to develop an understanding of how different things are connected. In this spirit, we do *not* want to present a seamless narrative. Rather we want you to pause regularly in the reading of these notes and work things out for yourselves. This is the role of problems, as well as some occasional asides. Thus, instead of collecting the problems at the ends of chapters, as many textbooks do, we embed the problems at their appropriate points in the text, encouraging you to stop and think, pick up a pen (or, as needed, put fingers to keyboard), and calculate. Some of the problems are small, essentially asking you to be sure that you understand something which goes by a bit quickly in the text. Others are longer, even open–ended, asking you to explore rather than to find a specific answer.

Students in our course should not be afraid of the large number of problems they find here! We will assign only a fraction of the problems in the weekly problem sets, which will be announced on the `blackboard` web site. The problems which we don't assign may nonetheless prove useful. Short problems could serve as warmup exercises for the assigned problems, while longer problems might serve as fodder for review as exam times approach. We take this opportunity to remind you that we encourage collaboration among the students in working on the problems, and more generally in learning the material of the course.

Authors

The freshman course evolved through discussions among many faculty. The lectures which form the basis for these notes on dynamics have been given in previous years by William Bialek, David Botstein, John Groves, Michael Hecht, Robert Prud'homme, Joshua Rabinowitz, Joshua Shaevitz and Ned Wingreen. Much has been added to the presentation by Michael Desai, Jeremy England, and Matthias Kaschube, who have led precepts. Because the problems play such a central role in the course, we especially thank all of those students who suffered through the early versions, and the succession of teaching assistants who have improved the problems as they prepared solution sets.

Contents

Chapter 0

Introduction

> La filosofia è scritta in questo grandissimo libro che continuamente ci sta aperto innanzi a gli occhi (io dico l'universo), ma non si può intendere se prima non s'impara a intender la lingua, e conoscer i caratteri, ne' quali è scritto. Egli è scritto in lingua matematica, e i caratteri sono triangoli, cerchi, ed altre figure geometriche, senza i quali mezi è impossibile a intenderne umanamente parola; senza questi è un aggirarsi vanamente per un'oscuro laberinto.
>
> G Galilei 1623

Galileo's remarks usually are paraphrased in English as "the book of nature is written in the language of mathematics." Indeed, one way to phrase the goal of physics is that we want to provide a concise and compelling mathematical description of nature, reading and summarizing the grand book to which Galileo refers. Literally the hope is that everything we see around us can be derived from a small set of equations. It is remarkable how much of the world has been "tamed" in this way: We really do know the equations that describe much of what happens around us, and in many cases we actually can derive or predict what we will see by starting with these equations and making fairly rigorous mathematical arguments. This is an extraordinary achievement.

We must admit, however, that much of what fascinates us in our immediate experience of the world remains untamed by mathematics. In particular, life seems much more complex than anything we find in the inanimate world, and correspondingly we suspect that it will be much more difficult to arrive at convincing mathematical theories of biological phenomena. To some extent this suspicion is correct, and our current understanding of biology is much more descriptive and qualitative than is our understanding of the traditional core areas of physics and chemistry. It is important to emphasize, however, that the conventional ways of teaching greatly exaggerate these differences. Thus one teaches physics and chemistry (especially to biologists) by presenting only the very simplest of examples, and one teaches biology by suppressing any role played by quantitative or theoretical analyses in establishing what we actually know. For a variety of reasons, it is time for this to change.

We live at an extraordinary moment in the history of science. From the large scale structure of the universe as a whole to the forces at work deep inside the atomic nucleus, we really can calculate what we will see when we look closely at the world around us. Emboldened by these successes, there is a widespread sense that our current qualitative descriptions of biological phenomena will be replaced by compelling mathematical theories that are tested and refined through sophisticated quantitative experiments and computational analyses, in parallel with our understanding of the inanimate world. These extraordinary scientific opportunities require a proportionately radical rethinking of our approach to undergraduate education, and this course is a first effort in this direction. Our goal is to present a more unified view of the sciences as a coherent attempt to discover and codify the orderliness of nature.

It should be clear that, in our view, the current divergence between the teaching of physics and the teaching of biology is a historical artifact which should be remedied. At the same time, the development of separate cultures in the different disciplines is something we should appreciate, respect, and try to understand. But we must always distinguish the current state of the culture from our ultimate goals. This distinction is not universally accepted. A distinguished 20th century biologist (who shall remain nameless here) also quotes Galileo, but he asserts that Galileo was limited to the science of his time, and since he didn't know much biology he of course couldn't realize that biology would be different, and presumably not mathematical. In contrast, we see no reason to doubt Galileo's original assertion that understanding ultimately will mean mathematical understanding.

When we first offered this course in the Fall of 2004, we thought that the goal of unification was so critical that we should stamp out any reference to the historical traditions of different disciplines. This now seems a little naive. Even if we agree that, as a community of scientists, we would like to arrive someday at a seamless understanding of both the animate and inanimate worlds, and that we want this understanding to be faithful to Galileo's vision, *today* the different disciplines are at very different points along this path. As a result, what a biologist sees as the development of a more quantitative biology can be quite different from what a physicist sees as the physics of life, and chemists would have yet a different view. These differences are interesting and important, and the tension among the advocates of the different points of view (perhaps even among your professors in this course!) is a creative tension. Thus, while we want to prepare you for a more unified view of the natural world, we want you to understand the context out which the next generation of scientific developments will come.[1] To do this, we start the course with three lectures that present three different viewpoints: from physics, from chemistry and from biology.

0.1 A physicist's point of view

The search for a compelling mathematical description of nature has led to the invention of new mathematical structures; indeed, starting with calculus, much of what we think of as advanced mathematics has its origins in efforts to understand nature. One way to organize our exploration is to identify the major classes of mathematical ideas that we use in thinking about the world, and this is the organization that we will follow in this course. But it makes sense to start by outlining the traditional content of a freshman physics course.

Classical mechanics. This is how we predict the trajectory of a ball when we throw it, and how we understand and predict the motions of the planets around the sun; at it's core are Newton's laws. If we broaden our view a bit to include the mechanics of fluids and solids, then this is also the branch of physics that governs biological motion on the scale of microns in and around cells; at the other end of the size scale, this is the physics that explains why planes can fly, why bridges support the weight of cars and trucks, and why the weather changes, sometimes unpredictably. In its original form, classical mechanics is *the* great example of describing the dynamics of the world in terms of differential equations, and it is for this purpose that calculus was invented.

---

[1] In addition, there is the practical fact that you continue your education not as 'integrated scientists' (whatever that might mean), but as physicists, chemists, biologists, engineers, ... We want to prepare students with a coherent introduction to the natural sciences that will serve them well no matter which discipline they choose for their major. Thus, this is emphatically *not* a physics or chemistry course for biology majors, but rather an alternative path into all of the majors. A few brave students have even used the course as a springboard to non–science majors, and one could argue that our integrated view is especially useful for people whose science education will end after their freshman year.

Figure 1: Not the mathematical tools we had in mind when we designed the course.

Thermodynamics and statistical physics. This part of our subject provides laws of astonishing generality, constraining what can and cannot happen even if we don't understand all the mechanistic details—e.g., the impossibility of perpetual motion machines. This also is the branch of physics that builds a bridge from the image of atoms and molecules whizzing about at random to the orderly phenomena that we see on a macroscopic scale. This is the physics of transistors and liquid crystals, of dramatic phenomena such as superconductivity and superfluidity, and even of the phase transitions that may have driven the extremely rapid expansion of our universe in its initial moments. Here the underlying mathematical structure is probabilistic: What we see in the world are samples drawn at random out of a probability distribution (as when we flip a coin or roll dice) and the theory specifies the form of the distribution.

Electricity and magnetism. It is a remarkable fact that objects seem to interact with each other over long distances, for example two magnets. In the 1800s these interactions were codified by thinking of each object as generating a *field* that pervades the surrounding space, and then the distant object responds to the field at its own location. Electric and magnetic fields are among the earliest examples of this sort of description, and eventually it was realized that the equations for these fields predict a dynamics of the fields themselves, independent their sources. This dynamics corresponds to propagating waves, much like the classical waves on the water's surface, but the velocity of propagation turned out to be the speed of light, and we now understand that light *is* an electromagnetic wave. Thus electricity and magnetism provides both a great example of how to describe the world in terms of fields and a dramatic example of unification among seemingly disparate phenomena, from the lodestone to the laser.

These three great divisions of our subject thus illustrate three different styles of mathematical description: Dynamical models in terms of differential equations, probabilistic models, and models where the fundamental variables are fields. One of the key ideas that we hope to communicate in this course is that these styles of mathematical description are applicable far beyond their origins. In particular, important parts of chemistry and physics share this underlying mathematical structure, and the same structures are applicable to the more complex phenomena of the living world. Thus instead of organizing our thinking around the historical divisions of physics, chemistry and biology, we will present our understanding of the world as organized by these mathematical ideas.

Dynamical models. Newton's laws predict the trajectories of objects as the solutions to differential equations. Strikingly similar differential equations arise in describing the kinetics of chemical reactions, the growth of bacterial populations, and the dynamics of currents and voltages in electrical circuits. Rather than just teaching these separate subjects, we want to give you an appreciation for the generality and power of these ideas as a framework for understanding dynamical phenomena in nature. We won't stop with the traditional examples, all carefully chosen for their simplicity, but will emphasize that the same approach describes complex networks of biochemical reactions in cells, the rich dynamics of electrical activity in neurons and networks, and so on. In order to meet these goals we will introduce as early as possible the art of approximation and the use of numerical methods as ways of getting both exact answers and better intuition.

Probabilistic models. Freshman physics and freshman chemistry each tackle the conceptually difficult problems of thermodynamics and the statistical description of heat. The mathematical models here are probabilistic—when we make measurements on the world we are drawing samples out of a probability distribution, and the theory specifies the distribution. But Mendelian genetics also is a probabilistic model, and related ideas permeate modern approaches to the analysis of large data sets. Starting with genetics, we will introduce the ideas of probability and proceed through a rigorous view of statistical mechanics as it applies to the gas laws, chemical equilibrium, etc.. Entropy will be followed from its origins in thermodynamics to its statistical interpretation, through its role in information theory and coding, highlighting the startling mathematical unity of these diverse fields. We will introduce the ideas of coarse–graining and approximation, explaining how the same formalism applies to ideal gases and to complex biological molecules.

Fields. While electromagnetism provides a compelling example of field dynamics, the coupled spatial and temporal variations in the concentration of diffusing molecules also generate simple field equations. These equations become richer as we include the possibility of chemical reactions. Surprisingly similar equations describe the migrations of bacterial populations in response to variations in the supply of nutrients, and related ideas describe problems in ecology, epidemiology and even economics (the e–sciences). Even simple versions of the reaction–diffusion problem have important implications for how we think about the emergence of spatial patterns (and, ultimately, body structure) in embryonic development. The dramatic prediction of light waves from the field equations of electricity and magnetism will lead us into an understanding of microscopes and X–ray diffraction, the experimental methods that literally allow us to see the inner working of matter and life.

Quantum mechanics. The themes of dynamics, fields and probability come together in the quantum world. Rather than a descriptive “modern physics” course, we will present a concise account of the Schrödinger equation, wave functions and energy levels, aiming at a rigorous derivation of atomic orbitals that provides a foundation for discussing the periodic table, the geometry of chemical bonding and chemical reactivity. At the same time we will present some of the compelling paradoxes of quantum mechanics, where we have a unique opportunity to discuss the sometimes startling relationship between mathematical models and experiment.

Reductionism vs. emergence

There is yet another way of organizing our exploration of scientific ideas, and this is the idea of reductionism. Roughly speaking, there is a view of physics and chemistry which says that we start with mechanics of the objects that we see around us, and then we start to take these apart to find out about their constituents. Once we discover that matter is made from molecules, and that molecules are built from atoms, we take apart the atoms to find electrons and the nucleus. Chemistry gives way to atomic physics, and then to nuclear physics as we try understand how the nucleus is built from its constituent parts, the protons and neutrons. Along the way we learn that protons and neutrons are not unique; if they smash into each other with enough energy we see many more particles, each with its own unique set of properties, and indeed many of these exotic particles occur naturally in cosmic rays that rain down on us constantly. Nuclear physics gives way to particle physics, and eventually we understand that the "subatomic zoo" can be ordered by imagining that there are yet more basic constituents called quarks; similarly the electron has several cousins in the zoo that are called leptons. The interactions among these particles are described by fields—just as in electricity and magnetism, and indeed there are profound mathematical connections among the equations for the electromagnetic field and the equations for the fields that mediate forces on this subatomic scale. Again the hope is for unification, and to a remarkable extent this has been achieved.

The march from atoms to quarks in one century is one of the great chapters in human intellectual history.[2] At the same time, describing physics *only* as the constant drive to peel away layers of description, searching for the 'fundamental' components of the universe, is a bit simplistic. In some circles this reductionist drive is emulated—trying to make some area of science "more like physics" often seems to mean making it more reductionist. At the same time, for many people "reductionist" is sort of a dirty word: Surely we must recognize that systems are more than the sum of their parts, and that essential functions are lost when we tear them to bits in the process of understanding them.

In fact, the portrait of physics as a strict reductionist enterprise misses about half of what physicists have been doing since $\sim$1950. The other half of physics is about how macroscopic or collective properties emerge from the interactions among more elementary constituents. A familiar (if, in the end, somewhat complicated) example is provided by water. We know that pure water is made from only one kind of molecule, and the essence of the reductionist claim is that the properties of water in a given environment (e.g., at some temperature and pressure) are determined by its molecular composition. As far as we know, this claim is true. Yet, at the same time, the most obvious properties of liquid water—it feels wet, and it flows—definitely are not properties of single water molecules. It's not even clear

---

[2] As new Princetonians, you can take pride in knowing that some of the important steps in this grand march took place right here.

that a small cluster with tens of molecules would have these properties; when we look at small numbers of molecules, for example, our attention is immediately drawn to the fact that there is a lot of empty space in between the molecules, while on a human scale this space is imperceptible and the water seems to be a continuous substance.

The discrepancy between single molecules and macroscopic properties is even greater if we think about solid water (ice). The statement that an ice cube is solid is a statement about rigidity: if we push on one side of the ice cube, the whole cube moves together, and in particular the opposite face of the cube also moves. This property can't even be defined for a single molecule, and it certainly isn't something that happens if we just have a few molecules. Indeed, it's not obvious why it works at all.

Imagine lifting a one kilogram cube of ice. You grip the edges, apply a force, and the entire block is raised by say one meter. In the process you have put about 10 Joules of energy into work against the force of gravity. This is more than enough energy to rip the first layers of water molecules off of the faces of the block, but that's not what happens. Instead of flying apart in response to the force, or flowing around your fingers like liquid water, all of the water molecules in the block of ice (even the ones that you're not touching!) move together. This rigidity or solidity of ice clearly has something to do with the water molecules, but clearly involves the whole block of material being something more than just the "sum of the parts."

Our whole language for talking about the block of ice or the flow of liquid water (or the flow of air—wind—in the atmosphere) is different from how we talk about molecules. Thus we can talk about a tornado as if it were an object moving across the globe, or about the hardness of the ice surface, and neither of these things correspond in a simple way to the things we might measure for individual molecules. Similar things happen in other materials, sometimes quite dramatically. Thus, while a single electron moving through a solid might rattle around, bumping into various atoms and eventually losing its way, when we cool that same hunk of metal down to very low temperatures, all the electrons can flow together in an electrical current that lasts essentially forever, a phenomenon called superconductivity. If each molecule in a liquid crystal display responded individually to applied electric fields, you could never get the bright and brilliant colors that you see on your laptop computer;[3] again there is some collective behavior in large

---

[3] Actually, this remark is slightly out of date, since many laptops now have thin film transistor displays. Liquid crystal displays still are fairly common for digital cameras, though.

groups of molecules, and the whole is more than the sum of the parts.

The understanding of how these sorts of macroscopic, collective behaviors emerge from the dynamics of electrons, atoms and molecules did not come in one bold stroke, as in the high school version of science history where Einstein writes down the theory of relativity and suddenly everything changes. Instead there were many independent strands of thought, which started to come together in the 1960s.[4] Gradually it became clear that, at least in a few cases, it was possible not just to understand that collective effects happen, not just to describe these more macroscopic dynamics, but even to understand how they can be derived, at least in outline, from something more microscopic. In this process, something remarkable happened: we understood that when macroscopic collective effects arise, once we focus on these effects we lose track of many of the microscopic details. The flow of a fluid provides a good example, since the equations which describe this flow depend on the density and viscosity of the fluid, and essentially nothing else. All of the complicated properties of the molecules—the geometry of their chemical bonds, their van der Waals interactions and hydrogen bonds with each other, ... —are irrelevant, except to set the values of those two parameters.[5] The 1970s brought even more dramatic examples of such 'universality,' building precise mathematical connections between seemingly completely different phenomena, such as the liquid crystals and superconductors mentioned above, but this is going too far for an introduction.

We'll come back explicitly to these ideas in the second half of the Fall semester, and more generally our discussion of statistical physics will be all about how to build up from the microscopic description of atoms and

---

[4] One of the landmarks was a lecture given in 1967 by our own Phil Anderson, published some years later: PW Anderson, More is different. *Science* **177,** 393–396 (1972). The piece was written partly in opposition to the notion that the reductionist search is somehow 'more fundamental' than the search for synthesis, and Phil's unique combative style comes through clearly in his writing. Sociology aside, this paper gives a beautiful statement of the idea hinted at above, that even our language for describing things evolves as we move from one level (e.g., molecules) to the next (fluids and solids). There can be independent discoveries of the relevant mathematical laws at each level, and it is by no means obvious how to move from one level to the next. Indeed, in those cases where we learn how to derive laws at one level from the dynamics 'underneath,' it is a great triumph.

[5] Actually one can do more. These parameters have units, and nobody tells you what system of units to use. By adjusting your system of units, you can almost make the parameters all be equal to one, so that there is truly nothing left of the molecular details. This isn't quite right, because there is still a dimensionless ratio of parameters that combines the properties of the fluid with the typical spatial scale and speed of the fluid flow, but this one number (Reynolds' number) tells the whole story. Flows with the same Reynolds' number look *quantitatively* the same no matter what molecules make up the fluid.

molecules to the phenomena that we observe on a human scale. Perhaps we can even give a hint of how the ideas of universality have given physicists the courage to write down theories for much more complex phenomena, up to the phenomena of perception and memory in the human brain. For now, however, enough philosophy.

The simplest models

All of the models mentioned above involve (at least) some calculus. But there is a much simpler class of model, maybe one that is so simple we don't even think of it is a "model of nature" in the grand sense that we use the word today—models in which one variable is just a linear function of the other. There are many familiar examples:[6]

- The voltage drop V across a resistor is proportional to the electrical current I that flows through the resistor, $V = IR$. This is Ohm's law, and R is the resistance.
- The force F that we feel when we stretch a spring is proportional to the distance x that we stretch it, $F = -\kappa x$. This is Hooke's law, and κ is called the stiffness of the spring.[7]
- The charge Q on a capacitor is proportional to the voltage difference V across the capacitor, $Q = CV$, where C is the capacitance.
- When an object moves through a fluid at velocity v, it experiences a drag force $F = -\gamma v$, where γ is called the drag or damping constant.
- The force of gravity is proportional to the mass of an object, $F = mg$ (this one is special!).

There are more examples, such as the fact that the rate at which your coffee cools is proportional to the temperature difference between the coffee and the surrounding air. While simple, there is a lot going on in these "laws."

First of all, the notion that these are "laws" needs some revisiting. Obviously if you take a rubber band and pull, then pull some more, eventually the rubber band will snap (don't blame me for the bruise if you feel compelled to verify this). Certainly when the band breaks Hooke's law stops

---

[6] Hopefully these are reminders of things you've learned in your high school course. If you miss one, don't worry, most will come back later in more detail.

[7] The symbol κ is the Greek letter "kappa," and (below) γ is "gamma," both lower case. It's incredibly useful to know the Greek alphabet; it's not hard, and if you find yourself in Athens you'll be able to read the street signs. See Fig 2.

Α	α	alpha	Ν	ν	nu
Β	β	beta	Ξ	ξ	ksi
Γ	γ	gamma	Ο	ο	omicron
Δ	δ	delta	Π	π	pi
Ε	ε	epsilon	Ρ	ρ	rho
Ζ	ζ	zeta	Σ	σς	sigma
Η	η	eta	Τ	τ	tau
Θ	θ	theta	Υ	υ	upsilon
Ι	ι	iota	Φ	ϕ	phi
Κ	κ	kappa	Χ	χ	chi
Λ	λ	lambda	Ψ	ψ	psi
Μ	μ	mu	Ω	ω	omega

Figure 2: The Greek alphabet: upper case, lower case, and the name of the letter. From `http://gogreece.about.com/`. We'll usually write the lower case sigma as σ. We'll try to avoid ι and o, because they are easily confused with i and o. By tradition, Δ and δ are used to indicate differences or changes, and we try to reserve ϵ for things that are small. Beyond these conventional choices, each subfield of science has its own conventions, and this can be a great source of confusion. If someone is explaining that in this particular problem, it's very important to know the value of ν, don't be afraid to ask "ν?".

being valid, but we suspect that the force stops being proportional to the distance we have stretched long before the band breaks. These considerations describe what happens when we stretch the rubber band, but of course we can also compress it, and then we know that it can go slack, so that no force is required to bring the ends together. See Fig 3. So in what sense is Hooke's law a law?

Statements such as Hooke's law and Ohm's law are very good approximations to the properties of many real materials, but they are not "laws" of universal applicability such as Newton's $F = ma$. But why do these approximations work? Let's think about some function, perhaps force as a function of length for the spring, or voltage as a function of current in a wire (resistor), etc.. Let's call this function $f(x)$. If you can see the whole function, it might be quite funny looking, as in Fig 4. On the other hand, if we only want to know the value of the function close to the place where $x = x_0$, we can make approximations (Fig 5).

We could start, for example, by ignoring the variations all together and saying that since x is close to x_0, we'll just pretend that the function is constant and equal to $f(x_0)$. A bit silly, perhaps, but maybe not so bad. The next best thing is to notice that you can fit a straight line to the function in the neighborhood of x_0, which is the same as writing

$$f(x) \approx f(x_0) + a(x - x_0), \tag{1}$$

where a is some constant that measures the slope of the line.

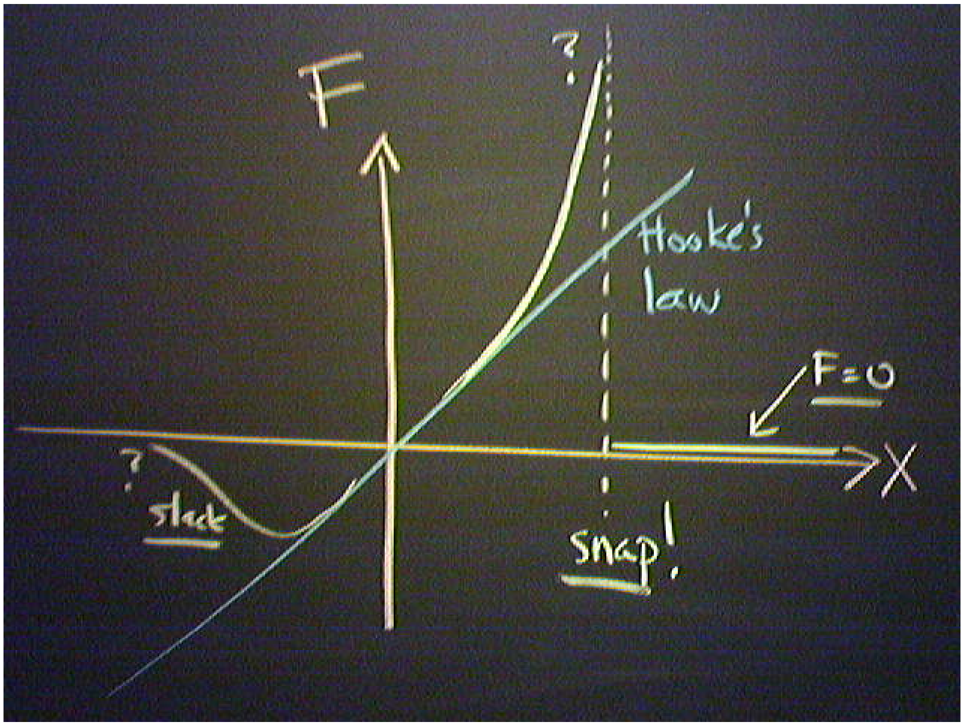


Figure 3: Force F that *opposes* lengthening of a rubber band, versus the length x of the band. Straight blue line indicates Hooke's law, $F = \kappa x$. At some critical length the band will snap; leading up to this it takes extra force, although it's not obvious exactly what happens, but after the snap it takes no force to move the ends apart since they're not connected (!). At the other side, once the rubber band shortens to the point of going slack, the force again goes to zero.

The next approximation would be to fit a curve in the neighborhood of x_0, starting with a parabola,

$$f(x) \approx f(x_0) + a(x - x_0) + b(x - x_0)^2. \tag{2}$$

Clearly we could keep going, using higher and higher order polynomials to try and describe what is going on in the graph. Notice that by writing our approximations in this way we guarantee that they give exactly the right answer at the point $x = x_0$.

Some of you will recognize that what we are doing is using the *Taylor series* expansion of the function $f(x)$ in the neighborhood of $x = x_0$. We recall

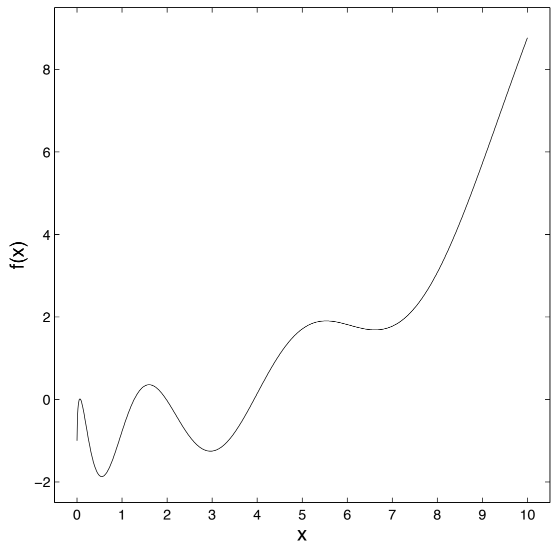


Figure 4: A function $f(x)$, chosen to have some interesting bumps and wiggles.

from calculus that for any function with reasonable smoothness properties, for some range of x in the neighborhood of x_0 we can write

$$\begin{aligned} f(x) &= f(x_0) + \left[\left. \frac{df(x)}{dx} \right|_{x=x_0} \right] \cdot (x - x_0) \\ &\quad + \frac{1}{2} \left[\left. \frac{d^2 f(x)}{dx^2} \right|_{x=x_0} \right] \cdot (x - x_0)^2 \\ &\quad + \frac{1}{3!} \left[\left. \frac{d^3 f(x)}{dx^3} \right|_{x=x_0} \right] \cdot (x - x_0)^3 + \cdots , \end{aligned} \tag{3}$$

where $\cdots$ are more terms of the same general form; we can write the same equation as

$$f(x) = f(x_0) + \sum_{n=1}^{\infty} \frac{1}{n!} \left[\left. \frac{d^n f(x)}{dx^n} \right|_{x=x_0} \right] \cdot (x - x_0)^n . \tag{4}$$

Now is a good time to be sure that you remember how to read and understand the summation symbol, as well as the vertical bar that means "evaluated at."

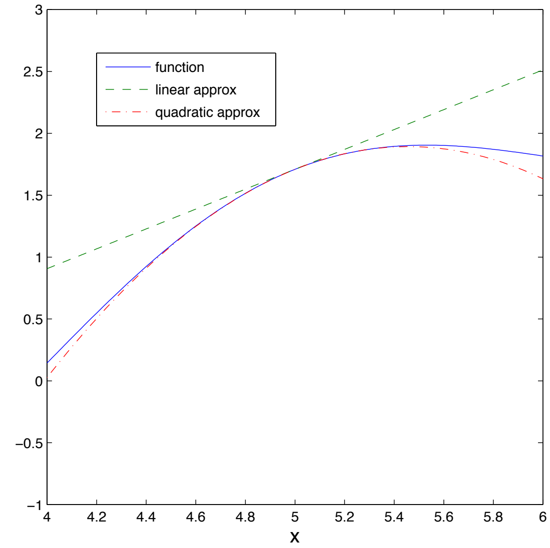


Figure 5: A closer view of the function $f(x)$ from Fig 4 in the neighborhood of $x = 5$, together with linear and quadratic approximations.

Problem 0: This might seem funny, but ... you should try reading Eq (4) out loud. It is very important that you be able to talk about you are doing when you solve problems, and that you come to see mathematics as integral to your description of the world. It's hard to do these things if you can't speak equations.

Figure 5 makes clear that the Taylor series works in a practical sense: We can start with a pretty wild function, and if we focus our attention on a small neighborhood then the first few terms of the Taylor series are enough to get pretty close to the actual values of the function in this neighborhood. Notice that this practical view is different from what you may have learned in your calculus class, where the emphasis is on proving that the Taylor series converges—that if we keep enough terms in the series we will eventually get as close as we want. The idea here is that just the first couple of terms are enough as long as we don't let $|x - x_0|$ get to be too big.

We can think of "laws" like Hooke's law or Ohm's law as the first terms in a Taylor series. Thus, as in Fig 3, the real relation between force and length (or voltage and current) might be quite complicated, but as long as we don't pull or push too much, the linear approximation works. But we haven't said what "too much" means. Look back at Fig 4. Although the function has lots of bumps and wiggles, they don't come very close together. Thus, as we sweep out a range of $\Delta x \in [-1, +1]$, things look pretty smooth. In fact Fig 5 focuses on a region of this size, and inside this region a low order approximation indeed works very well. So we understand that the first terms of a Taylor series are enough if we look at a range of x that is smaller than some *natural scale* of variations in the function we are trying to approximate.

A key point in physical systems is that the "natural scale" we are looking for has units! When we say that Hooke's law is valid if we don't stretch the spring too much, how far is too much corresponds to some real physical distance. What is this distance? Similarly, when we pass current through a wire, we say that Ohm's law is valid if we don't try to use too much current or apply too large a voltage ... but what is the natural scale of current that corresponds to "too much"? Being able to answer these questions is a critical step in thinking quantitatively about the natural world, and we will return to these problems several times during the course.

Problem 1: In order to answer questions about the "natural scale" for different phenomena, you will need to think about orders of magnitude. It might be hard to explain why something comes out to be exactly 347 (in some units), but you should be able to understand why it is ~ 300 and not ~ 30 or ~ 3000. Indeed, sometimes it's more satisfying to have a short argument for the approximate answer than a long argument for the exact answer.

(a.) What is the typical distance between molecules in liquid water? You should start with the density of water, $\rho = 1\,\text{gram/cm}^3$.

(b.) Many bacteria are roughly spherical, with a diameter of $d \sim 1\,\mu\text{m}$. If you divide up the weight of the bacterium, you find that it is 50% water, 30% protein, and 20% other molecules (e.g., RNA, DNA, lipid). A typical protein has a molecular weight of 30,000 atomic mass units (or Daltons).[8] Roughly how many protein molecules make up a bacterium? A typical bacterium has genes that code for about 5,000 different proteins. On average, how many copies of each protein molecule is present in the cell?

(c.) In [b] you computed an average number of copies for all proteins, but different proteins are present at very different abundances inside the cell. Indeed, there are important proteins (such as the transcription factors that help to turn genes on and off) that

---

[8] Recall that one atomic mass unit is a mass of one gram per mole.

function at concentrations[9] of $\sim 1-10\,\mathrm{nM}$. How many molecules of these proteins are present in the cell?

(d.) To encourage this kind of thinking, Enrico Fermi famously asked "How many piano tuners are there in America?" during a PhD exam in Physics. Similar questions include: How many students enter high school in the United States each year? How many college students each year need to become teachers in order to educate all these people? How many houses does the tooth fairy visit each night?[10] Answer these questions, and formulate one of your own.

Problem 2: If we have a block of material with area A and length L, then the stiffness for stretching or compressing along its length will be $\kappa = YA/L$, where Y is called the Young's modulus.

(a.) Explain why the stiffness should be proportional to the area and inversely proportional to the length of the block.

(b.) Show that Y has units of an energy density (or energy per unit volume—joules/m^3 or erg/cm^3). Note that this makes sense because the energy[11] that we store in the block when we stretch it by an amount ΔL, $E_{\mathrm{stored}} = (1/2)\kappa(\Delta L)^2$, works out to be proportional to the volume ($V = AL$) of the block:

$$E_{\mathrm{stored}} = \frac{1}{2}\kappa(\Delta L)^2 = \frac{1}{2}Y\cdot(AL)\cdot\left(\frac{\Delta L}{L}\right)^2. \tag{5}$$

(c.) Diamond is one of the stiffest materials known, and it has $Y \sim 10^{12}\,\mathrm{N/m^2}$ (or $\mathrm{J/m^3}$). The density of diamond is $\rho = 3.52\,\mathrm{g/cm^3}$. Convert Y into an energy per carbon atom in the diamond crystal. How does this compare with the energy of the chemical bonds in the diamond crystal? Note that you'll need to look up this number . . . be careful about units! Does your answer make sense?

Problem 3: Going back to the *E coli* in Problem 1, we want to understand the implications of the fact that one bacterium can make a complete copy of itself (dividing into two bacteria) in $\tau \sim 20\,\mathrm{min}$.

(a.) Proteins are synthesized on ribosomes, which can add ~ 20 amino acids per second to a growing protein chain. If the typical protein has 300 amino acids, how many protein molecules can one ribosome make within the doubling time τ?

(b.) In order to double within τ, the bacterium presumably has to make an extra copy of all of its protein molecules. How many ribosomes does it need in order to do this? Make use of your results from Problem 1 on the numbers of protein molecules per cell.

(c.) The ribosome is quite large as molecules go, with a diameter of $\sim 25\,\mathrm{nm}$. If you could cut open the bacterium and see all the ribosomes, how far apart would they be? Is there much empty space between the ribosomes, or is the cell's interior more densely packed?

---

[9] M is the abbrevation for Molar, or moles per liter. The little n stands for nano–; recall that milli $= 10^{-3}$, micro $= 10^{-6}$, nano $= 10^{9}$, pico $= 10^{-12}$, femto $= 10^{-15}$, and (you might not have heard this one) atto $= 10^{-18}$. Thus, nM denotes a concentration of 10^{-9} moles per liter.

[10] Admittedly, this is a bit more hypothetical than Fermi's problem.

[11] Here we ask you to recall from high schol that when you stretch a spring of stiffness κ by a distance x, the energy that you store in the spring is $\kappa x^2/2$. If you don't remember this, don't worry; we'll come back and derive it later in the course.

It would be wrong to leave this discussion of very simple models without talking about one of the very simplest—so simple, in fact, that from our modern perspective we can miss that it is a model at all. You all know that

$$2\mathrm{H}_2 + \mathrm{O}_2 \rightarrow 2\mathrm{H}_2\mathrm{O}. \tag{6}$$

We talk about this equation in terms of each water molecule being made out of two hydrogen atoms and one oxygen atom. But not so long ago, we didn't know about atoms. What we did know was that if you mix hydrogen and oxygen together, you get water. When people looked more carefully, they found that this could be made quantitative: A certain amount of hydrogen and oxygen, in certain proportions, are needed to make a certain amount of water. But "amounts" are measured in some units which, from our modern point of view, are rather arbitrary—liters (or worse, gallons) of the gases, grams of the liquids or solids, ... So you might learn that some number of liters of hydrogen gas plus some number of liters of oxygen gas produces some number of grams of liquid water.

$$\begin{aligned} &44.8 \text{ liters hydrogen gas} \quad + \quad 22.4 \text{ liters oxygen gas} \\ &\qquad\qquad\qquad\qquad \rightarrow 36 \text{ milliliters liquid water.} \end{aligned} \tag{7}$$

Now you do other experiments, mixing hydrogen and oxygen with other materials. Each time there is some rule about how the different amount combine. It really was an amazing discovery that if you choose your units correctly you can turn all these funny numbers [as in Eq (7)] into the integers of Eq (6). Thus, if you say that one unit of gas at room temperature and pressure is 22.4 liters, then all of the reactions involving gases simplify, and so on.

What's going on here? Now we know, of course, that we should measure the number of molecules or the number of moles of each substance, and then the rule for combining macroscopic quantities just reflect the rules for combining individual atoms. But we can think about trying to write down the rules for the macroscopic quantities alone, and then these are simple functional relations—in fact they are linear relations, not unlike Hooke's law. The wonderful thing is that the coefficients in these linear relations don't take on arbitrary values (as with the stiffness of a spring) but if we choose our units correctly these coefficients are just pure numbers. It took a long time to go from this discovery to the modern view of atoms and molecules, but when you find that there is a way of looking at the world in which the numbers you need to know are integers, you know you're on to something!

What physicists do

After all of this, you might still be confused about what physicists do, today. The dividing up of our intellectual explorations into different disciplines is a human endeavor, and so to some extent this (as with parallel questions about chemistry, biology, other sciences, as well the humanities) is a sociological question. It might be worth pointing out, however, that disciplines have a choice to define themselves by the objects that they study, or by the kinds of questions that they ask. To give an example far from the sciences, one might wonder whether one should study film in the English department. If by the discipline of "English" one means "studying books written in English," then obviously you don't study film. If, on the other hand, one understands "English" to mean the exploration of certain kinds of questions about the interaction of language and culture among English speaking peoples, then film is fair game. In this spirit, it seems fair to say that, perhaps more than most scientific fields, physics is defined by the kinds of questions that physicists ask.

Physicists really are interested in fulfilling the Galilean image of reading the book of Nature, and we fully expect it to be a short book once we have the right language. As mentioned at the outset, there are many natural phenomena for which we have a reasonable mathematical description, corresponding perhaps to well defined chapters in the book. Revisiting these (more or less) known chapters is fun, but more of the community is excited about the places where (to strain the metaphor) the text is incomplete. There are two very different ways in which this can happen.

In one class of problems, we're pretty sure we know the right mathematical description—essentially because the description comes in many parts, and each part has been tested in some detail—but there are broad classes of phenomena that should come out of this description and we don't know how to make the connection. This happens across many different scales, from the nucleus to the weather. Although faster computers certainly help, many of these problems require us to inject new ideas even to make direct computation of the answer (let alone understanding the answer) feasible.

A very different possibility is to go to extremes, to the more literal edges of our understanding. Thus, thousands of physicists are working together on two experiments in Geneva that will probe the structure and dynamics of matter on a scale millions of times smaller than the atomic nucleus. At the opposite extreme, physicists and astronomers[12] are trying to survey the

---

[12] The boundary between physics and astronomy is not always so easy to define. The question of whether a university has separate physics and astronomy departments, for

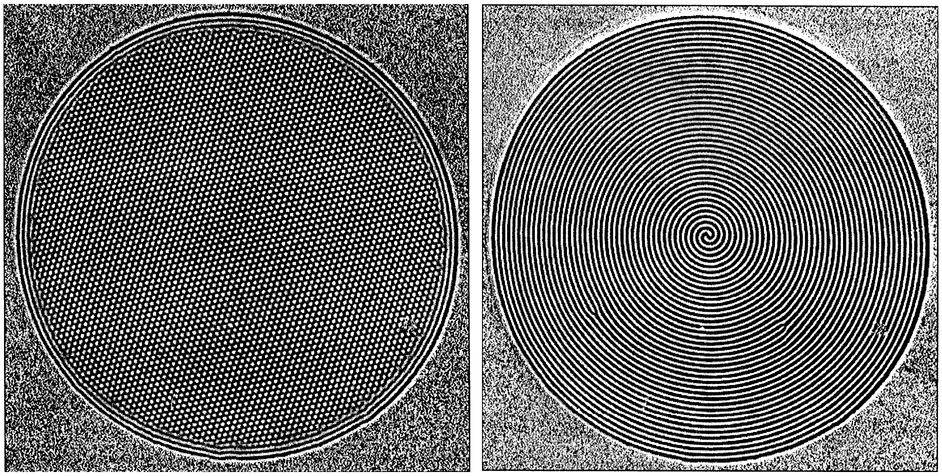


Figure 6: What you see at left looks like a perfect crystal of beads, but this actually is a small ($\sim 10\,\mathrm{cm}$ diameter) container filled with carbon dioxide at high pressure, and heated from below. The image is formed by passing light through the gas, sometimes called a 'shadowgraph.' The structure of image is sensitive to the patterns of temperature, because changing the temperature of a gas causes a change in refractive index, bending the rays of light and casting shadows. At right, the same container of gas, but with a slightly different amount of heating. Other than the high pressure, there is nothing extreme in the conditions—temperatures on both the top and bottom of the container are near room temperature. What is true is that these temperatures are held very constant (to within a few thousandths of a degree) so that the patterns will not be disrupted by variations in conditions; similarly, the top and bottom of the container are extremely flat (smooth to within the wavelength of light), and the whole system is held horizontal with high precision so that the direction of gravity is aligned with axis of symmetry through the center of the circle. Despite the fact that conditions are constant, the spiral patterns actually rotates slowly during the experiment. From E Bodenschatz, JR de Bruyn, G Ahlers & DS Cannell, *Physical Review Letters* **67,** 3078–3081 (1991).

structure of the universe on the largest possible scales, and to understand the way in which this structure has evolved over the billions of years since the big bang.

Extremes can be more subtle. Thus, for example, we usually think that the mysteries of quantum mechanics are confined to the scale of atoms, and last for proportionately short times. Can we stretch the weirdness out to a more human scale? Are there fundamental, or only practical, limits

---

example, is almost always a question of history. "Astrophysics" seems like a sensible blending of the different fields, but there are excellent universities that have departments with names like "astronomy and astrophysics" that are separate from the physics department. All terribly confusing.

on our ability to do this? This is not just a question of principle, since if we could harness the quantum properties of matter on the right scale, we could build computers that are qualitatively more powerful than todays digital machines. At present such actual 'quantum computers' are the stuff of fiction, but quantum computing, and the surrounding questions of how we control the dynamics of quantum systems, is a major research topic.

Another boundary of our understanding, which could be thought of as a combination of our two major categories, concerns complexity and organization. We know that if we put many atoms or molecules in a box, they organize themselves in interesting ways. There are solids, liquids and gases, but also more refined categories—such as solids that conduct electricity (or not), or which act as magnets, and so on. Perhaps surprisingly, it's not clear that we even have a complete catalog for these "states of matter," let alone a framework within which we can understand why the different states emerge from different combinations of atoms and external conditions. Especially intriguing are those cases where matter organizes itself in more complex ways, as often happens in response to a continual flow of energy through the system. Examples along this line of thinking start with very simple cases, such as the beautiful patterns that form in the flow of a fluid layer heated from below (Fig 6). The most distant reach along this path of self–organization into complex states is, of course, life itself.

0.2 A chemist's point of view

0.3 A biologist's point of view

[These sections remain to be written. Current students should see the less formal notes posted to `blackboard`.]

Chapter 1

Newton's laws, chemical kinetics, ...

When you look around you, you see many things changing in time. Our most powerful tools for describing such dynamics are based on differential equations. This mathematical approach to the description of nature started with mechanics, and grew to encompass other phenomena. In this section of the course, we'll introduce you to these ideas using what we think are the simplest examples. Following the historical path, we'll begin with mechanics, but we'll quickly see how similar equations arise in chemical kinetics, electric circuits and population growth. Sometimes the simple equations have simple solutions, but even these have profound consequences, such as understanding that most of the chemical elements in our solar system were created at some definite moment several billion years ago. In other cases simple equations have strikingly complex solutions, even generating seemingly random patterns. This is just a first look at this whole range of phenomena.

1.1 Starting with $F = ma$

By the time you arrive at the University, you have heard many things about elementary mechanics. In fact, much of what we cover in these first lectures are things you already know. We hope to emphasize several points: First, many of the things which you have may have remembered as isolated facts about the trajectories of objects really all follow from Newton's laws by direct calculation. Next, you need to take seriously the fact that Netwon's $F = ma$ is a differential equation. Finally, hidden inside some elementary facts that you learned in high school are some remarkably profound truths about the natural world. We won't have a chance to discuss their consequences, but we'd like to give you some flavor for these advanced but fundamental ideas.

Let us begin with Newton's famous equation,

$$F = ma. \tag{1.1}$$

At the risk of being pedantic, let's be sure we know what all the symbols mean. We all have an intuitive feeling for the mass m, although again we'll see that there is something underneath your intuition that you might not have appreciated. Acceleration is the clearest one: We describe the position of a particle as a function of time as $x(t)$, and the then the velocity

$$v(t) = \frac{dx(t)}{dt} \tag{1.2}$$

and the acceleration

$$a(t) = \frac{d^2x(t)}{dt^2}. \tag{1.3}$$

As a warning, we'll sometimes write dx/dt and sometimes $dx(t)/dt$. These two ways of writing things mean the same thing; the second version reminds us that we are talking not about variables but about *functions*—algebra is about equations for variables, but now we have equations for functions. Alternatively we can say that equations like $F = ma$ are statements that are true at every instant of time, so really when we write $F = ma$ we are writing an infinite number of equations (!). This may not make you feel better.

We have defined all the terms in Newton's famous Eq, (1.1)—all except for the force F. The definition of force is a minor scandal.[1] As far as I know, there is no independent definition of force other than through $F = ma$. If you want to go out and measure a force you might arrange for that force to stretch a spring, then look how far it was stretched, and if you know the spring constant you can determine the force. But how did you measure the spring constant? You see the problem.

In effect what Newton did was to say that when we observe accelerations we should look for explanations in terms of forces. This embodies the Galilean notion of inertia, that objects in motion *tend to keep moving* and hence if they change their velocity there should be a reason. If it turns out

---

[1] See, for example, F Wilczek, Whence the force of $F = ma$? I: Culture shock, *Physics Today* **57,** 11–12 (2004); `http://www.physicstoday.org/vol-57/iss-10/p11.html`.

that forces are arbitrarily complicated, then we're in deep trouble. In this sense, $F = ma$ is a framework for thinking about motion, and its success depends on whether the rules that determine the forces in different situations are simple and powerful.

Leaving aside these difficulties with the definition of force, Newton's law becomes a differential equation

$$m\frac{d^2x(t)}{dt^2} = F. \tag{1.4}$$

To build up some intuition, and some practice with the mathematics, we will start with three simple cases: zero force, a constant force, and a force that is proportional to velocity. Of course these are not just simple examples, they actually correspond to situations that are fairly common in the real world and that you will study in the laboratory. Again you probably know much of will be said here, but it's worth going through carefully and being sure you understand how it emerges from the differential equation.

These problems are designed to make you comfortable, once again, with the ideas from calculus that we will need in the next sections.

Problem 4: In Fig 1.1 we plot the velocity vs time $v(t)$ for an object moving in one dimension. Sketch the corresponding plots of position $x(t)$ and acceleration $a(t)$ vs time. If you need additional assumptions, please state them clearly. Be careful about units.

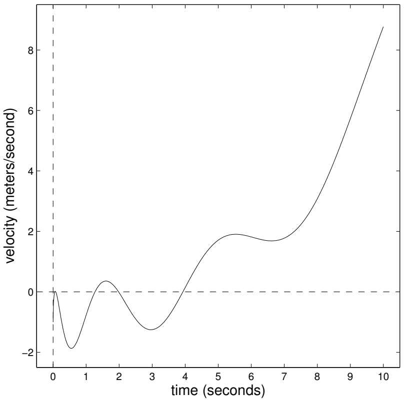


Figure 1.1: Velocity vs time for some hypothetical particle.

We are going to use MATLAB repeatedly in the course. Princeton students can go to `http://www.princeton.edu/licenses/software/matlab.xml` to find out about how to get started with their own computers; we'll also make sure that you get access to local computers that have MATLAB running on them. Hopefully, this problem is a good introduction. Note that you can type `help command` to get MATLAB to tell you how things work; for example, `help plot` will tell you something about those mysterious symbols such as `k--` below.

Problem 5: In fact the funny looking plot in Fig 1.1 corresponds to

$$v(t) = \sin(2\pi\sqrt{t}) + \left(\frac{t}{5}\right)^3 - \exp(-t/4). \tag{1.5}$$

(a.) Find analytic expressions for the position and acceleration as functions of time. You may refer to a table of integrals (or to its electronic equivalent), but you must give references in your written solutions.

(b.) Use MATLAB to plot your results in [a]. To get you started, here's a small bit of MATLAB code that should produce something like Fig 1.1:

```
t = [0:0.01:10];
v = sin(2*pi*sqrt(t)) + (t/5).^3 - exp(-t/4);
figure(1)
plot(t,v); hold on
plot([-1 11],[0 0],'k--',[0 0], [-3 10],'k--');
hold off
axis([-0.5 10.5 -2.5 9.5])
```

There are just two lines of math, and the rest is to make the graph and have it look nice. How do these plots compare with your sketches in the problem above?

Zero force

When there are no forces, $F = 0$, Eq (1.4) becomes

$$m\frac{d^2x(t)}{dt^2} = 0. \tag{1.6}$$

Notice that this equation, as always with differential equations, is telling us about how things change from moment to moment. If we imagine knowing where things start, we should be able add up all the changes from this starting point (which we can call $t = 0$) until now (t). In this simplest of cases, "adding up all the changes" really is a matter of doing integrals.

Although professors sometimes forget this, it's important to be careful about limits when you do integrals. In this case, we want to know how things evolve from a starting moment until now, so all integrals should be definite integrals from some initial time $t = 0$ up to now (t). Going carefully through the steps

$$\begin{aligned}
m\frac{d^2x(t)}{dt^2} &= 0 \\
\int_0^t dt\, m\frac{d^2x(t)}{dt^2} &= \int_0^t dt\,[0] && (1.7) \\
m\int_0^t dt\frac{d^2x(t)}{dt^2} &= \int_0^t dt\,[0] && (1.8) \\
m\left[\left.\frac{dx(t)}{dt}\right|_t - \left.\frac{dx(t)}{dt}\right|_{t=0}\right] &= 0 && (1.9) \\
\frac{dx(t)}{dt} &= \left.\frac{dx(t)}{dt}\right|_{t=0} && (1.10) \\
\frac{dx(t)}{dt} &= v(0). && (1.11)
\end{aligned}$$

You should get in the habit of following these derivations with a pen in your hand, not just reading. Whenever we go through a long series of steps, you have to ask yourself both (a) if you understand where we are going and why, and (b) if you understand how we take each step. Near the start of the course, it seems best to lead you in this process, but by the end you should be doing it yourself. So, in this case, let's see how each step worked:

Eq (1.7) → (1.8) Since the mass m doesn't change with time (in this problem!) you can take it outside the integral.

Eq (1.8) → (1.9) Taking the integral of zero gives zero, while taking the integral of a derivative gives back the function itself.

Eq (1.9) → (1.10) Since the mass isn't zero, we can divide it through, and then rearrange.

Eq (1.10) → (1.11) Finally, since dx/dt is the velocity, we call $dx/dt|_{t=0} = v(0)$, the initial velocity.

What we have shown so far is that the velocity at time t is the same as at time $t = 0$: Objects in motion stay in motion, as promised.

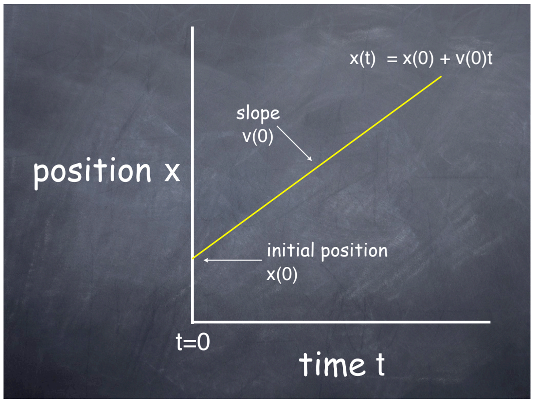


Figure 1.2: Trajectory of an object moving with zero force, from Eq. (1.14). Position vs. time is a straight line, with a slope equal to the initial velocity and an intercept equal to the initial position.

Now we go further, integrating once more:

$$\begin{aligned}
\frac{dx(t)}{dt} &= v(0) \\
\int_0^t dt \frac{dx(t)}{dt} &= \int_0^t dt\, v(0) && (1.12) \\
x(t) - x(0) &= v(0)t && (1.13) \\
x(t) &= x(0) + v(0)t. && (1.14)
\end{aligned}$$

What this shows is that if we plot position vs. time, we should find a straight line, as shown in Fig 1.2.

An important thing to remember is that position and force really are vectors. Thus if the (vector) force is equal to zero, then there is an equation like Eq (1.14) along each direction. As an example, in two dimensions we might write

$$\begin{aligned}
x(t) &= x(0) + v_x(0)t && (1.15) \\
y(t) &= y(0) + v_y(0)t. && (1.16)
\end{aligned}$$

This is important, because the plot of x vs. t (which is what we solve for most directly!) is not what you see when you watch things move. What you actually see is something more like y vs. x as the object moves through space. In this case, if you plot $y(t)$ vs. $x(t)$, you get a straight line. You can see this by a little bit of algebra:

$$\begin{aligned} x(t) &= x(0) + v_x(0)t \\ x(t) - x(0) &= v_x(0)t \qquad (1.17) \\ \frac{x(t) - x(0)}{v_x(0)} &= t \qquad (1.18) \\ \Rightarrow y(t) &= y(0) + v_y(0)t = y(0) + v_y(0) \cdot \frac{x(t) - x(0)}{v_x(0)} \qquad (1.19) \\ y(t) &= \frac{v_y(0)}{v_x(0)} x(t) + \left[y(0) - \frac{v_y(0)}{v_x(0)} x(0) \right], \qquad (1.20) \end{aligned}$$

and we recognize Eq (1.20) as the equation for a line with slope $v_y(0)/v_x(0)$. So motion without forces is motion at constant velocity, but also motion in a straight line.

Constant force

The standard example of motion with a constant force is the effect of gravity here on earth. This is a slight cheat, since of course the gravitational pull should depend on how far we are from the center of the earth. But if we do our experiments in a room (even a large room) it's hard to change this distance by more than a few meters, while the radius of the earth is measured in thousands of kilometers, so the changes in distance are only one part in a million. One can measure forces with enough accuracy to see such effects, but for now let's neglect them.

So, in the approximation that we don't move too far, and hence the pull of the earth's gravity is constant, we write

$$F = -mg, \qquad (1.21)$$

with the convention that x is measured upward; thus the downward force of gravity is negative, as shown in Fig 1.3. Putting this together with $F = ma$, we have

$$m \frac{d^2 x(t)}{dt^2} = -mg. \qquad (1.22)$$

The extraordinary thing is that the mass m appears on both sides of the equation, so we can cancel it, leaving

$$\frac{d^2 x(t)}{dt^2} = -g. \qquad (1.23)$$

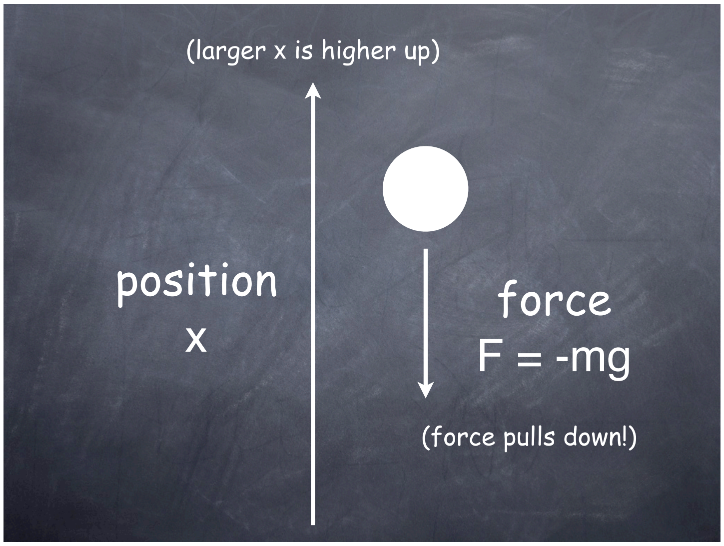


Figure 1.3: A particle moving under the influence of gravity, as in Eq (1.22).

Now in this equation, $x(t)$ denotes the position of the object, and g is a property of the earth—none of the properties of the object appear in the equation! Even without solving the equation we thus make the prediction that all objects should fall toward the earth in exactly the same way, and this is what Galileo famously is supposed to have tested by dropping different objects from the Tower of Pisa and finding that they hit the ground at the same time.

The statement that every object falls in the same way obviously is wrong, as you know by watching leaves float and flutter to the ground. The idea is that all these differences arise from forces exerted by the air, and so if we could take these away and "purify" the effects of gravity we would really would see *everything* fall in the same way.[2] A number of science museums have beautiful demonstrations of this, with long tubes out of which they can pump all the air and then drop either a rock or a feather. Even if you know the principles it is pretty compelling to see a feather drop like a rock!

One might be tempted to think that our ability to cancel the masses in Eq (1.22) is an approximation. Perhaps. But in the 1950s here at Princeton, Robert Dicke and his colleagues did an amazing experiment to show that this approximation is accurate to about 11 decimal places. This certainly

---

[2] One should take a moment to appreciate Galileo's insight, separating these effects in his mind in advance of methods for doing the experiments.

makes us think that what we have here is not an approximation but really something that one can call a law of nature.

Just so that you know all the words, the mass which appears in $F = ma$ is called the *inertial mass*, since this is what determines the inertia of an object. Inertia expresses the tendency of objects to keep moving in the absence of forces, and corresponds intuitively to the effort that we have to expend in stopping of deflecting the object. We also use inertia in everyday English to mean something quite similar, although not only in reference to mechanics. In contrast, the mass in $F = -mg$ is called the *gravitational mass*, for more obvious reasons. The statement that the masses cancel thus is the "equivalence of gravitational and inertial masses," or simply the "principle of equivalence."

The essential content of the principle of equivalence is clear from Eq (1.23): You actually can't tell the difference between a little extra acceleration (on the left hand side of the equation) and slightly stronger gravity (on the right). Einstein made the point in a thought experiment, imagining himself trapped in an elevator. Unable to see outside, he argued that he couldn't tell the difference between falling freely in a gravitational field and being accelerated (e.g. by rocket jets attached to the elevator). From the Newtonian point of view, this equivalence is a coincidence. After all, there are other forces such as electricity and magnetism which aren't proportional to mass, and thus one could have imagined that the gravitational force wasn't proportional to mass either. Indeed, you may remember that when we go beyond the approximation of gravity as a constant force, if two objects with masses m_1 and m_2 are a distance r apart, then the force that one objects exerts on the other is given by

$$F = -\frac{Gm_1m_2}{r^2}, \tag{1.24}$$

where the minus sign indicates that the force is attractive, and G is a constant (called Newton's constant). This is very much like Coulomb's law for the force between two particles with charges q_1 and q_2, again separated by a distance r,

$$F = \frac{q_1q_2}{r^2}. \tag{1.25}$$

Thus, except for the constant, the masses act like "gravitational charges," and it's a mystery why the gravitational charge[3] should be the same as the mass in $F = ma$.

---

[3] Another point worth noting concerns the sign of the force. Electrical charges can be

In 1905, Einstein wrote a series of papers that shook the world—on what we now call the special theory of relativity, on the idea that light is quantized into photons, and on Brownian motion and the size of atoms. Fresh from these triumphs, he decided that the mysterious coincidence between inertial and gravitational masses was a central fact about nature, indeed *the* central fact that needed his attention, and he set out to construct a theory of gravity in which the principle of equivalence is fundamental. It took him a decade, but the result was the general theory of relativity, arguably the greatest among his many great achievements. As you may have heard, general relativity involves a radical rethinking of our ideas about space and time and predicts the existence of black holes, the expansion of the universe, and other astonishing (but true!) things. We aren't ready for all this ... so reluctantly we will go back to the more mundane falling of things to the ground. But for now we'd like you to remember that when you read about the black hole in the center of our galaxy, the theory which predicts the existence of these exotic objects grew out of Einstein's taking *very* seriously a seemingly simple and obvious coincidence in the physics of everyday objects.

So, back to Eq (1.23). By now it should be clear what to do—integrate twice, as in the case of zero force:

$$\begin{aligned}
\frac{d^2x(t)}{dt^2} &= -g \\
\int_0^t dt\,\frac{d^2x(t)}{dt^2} &= \int_0^t dt\,[-g] && (1.26)\\
\frac{dx(t)}{dt} - \left.\frac{dx(t)}{dt}\right|_{t=0} &= -gt && (1.27)\\
\frac{dx(t)}{dt} &= \left.\frac{dx(t)}{dt}\right|_{t=0} - gt && (1.28)\\
\frac{dx(t)}{dt} &= v(0) - gt && (1.29)\\
\int_0^t dt\,\frac{dx(t)}{dt} &= \int_0^t dt\,[v(0) - gt] && (1.30)\\
x(t) - x(0) &= v(0)t - \frac{1}{2}gt^2 && (1.31)\\
x(t) &= x(0) + v(0)t - \frac{1}{2}gt^2. && (1.32)
\end{aligned}$$

---

positive or negative, and from Eq (1.25) we see that oppositely signed charges attract, while similarly signed charges repel one another. In contrast, because the gravitational charge is equal to the mass, and all the masses that we experience in everyday life are positive, all objects attract one another.

Thus we recover the $\frac{1}{2}gt^2$ that you all remember from high school.

Once again, $x(t)$ is not something you literally "see," since it is what you get by plotting position vs. time. On the other hand, position and force are both vectors, as noted above, but gravity only acts along one dimension (up/down). So if x is the up/down direction and y is measured parallel to the surface of the earth—opposite the usual convention!—then x obeys Eq (1.32) while y obeys Eq (1.14):

$$\begin{aligned} x(t) &= x(0) + v_x(0)t - \frac{1}{2}gt^2 && (1.33) \\ y(t) &= y(0) + v_y(0)t. && (1.34) \end{aligned}$$

But nobody told you where you should put $y = 0$, so you might as well choose this point so that $y(0) = 0$. Then the position y is proportional to t, and hence plotting x vs. y is just like plotting x vs. t except for the units on the horizontal axis. Thus one of the nice things about the trajectories of objects in our immediate environment is that distance parallel to the earth provides a surrogate for time, and we can literally see the trajectories played out in front of us. In particular, this means that when you throw something it follows a parabolic trajectory.

It's worth going through the algebra of the parabolic trajectory, choosing $y(0) = 0$ as suggested:

$$\begin{aligned} y(t) &= v_y(0)t && (1.35) \\ t &= \frac{y(t)}{v_y(0)} && (1.36) \\ x(t) &= x(0) + v_x(0)t - \frac{1}{2}gt^2 = x(0) + v_x(0)\frac{y(t)}{v_y(0)} - \frac{1}{2}g\left[\frac{y(t)}{v_y(0)}\right]^2 && (1.37) \\ x &= x(0) + \left[\frac{v_x(0)}{v_y(0)}\right]\cdot y - \left[\frac{g}{2v_y^2(0)}\right]\cdot y^2. && (1.38) \end{aligned}$$

I hope it's clear that this is a parabola.

Standard questions at this point are of the following sort: How far along the y axis does the object go before hitting the ground? To answer this question you choose the ground to be at $x = 0$ and solve for the value of $y = y_{\text{hit}}$ that results in $x = 0$. This is especially simple if the object *starts* at $x = 0$, which kind of makes sense if you fire a rocket off the ground (see

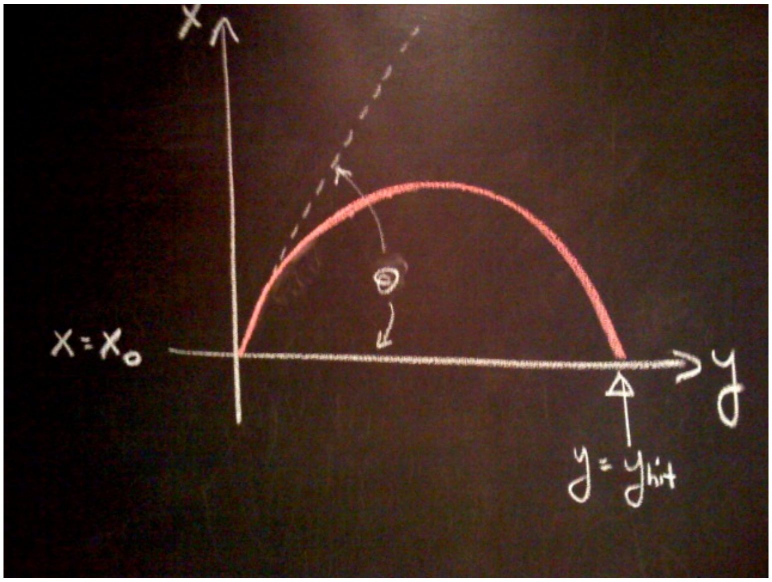


Figure 1.4: Launching an object from the ground. Initial position is $[x(0), y(0)]$, chosen for convenience as $(0, 0)$. Initial velocity launches the object in a direction θ, and the object returns to $x = 0$ at some point y as in Eq. (1.44).

Fig 1.4). Then $x(0) = 0$, and the condition $x = 0$ is equivalent to

$$\begin{aligned} 0 &= \left[\frac{v_x(0)}{v_y(0)}\right] \cdot y_{\text{hit}} - \left[\frac{g}{2v_y^2(0)}\right] \cdot y_{\text{hit}}^2 && (1.39) \\ &= y_{\text{hit}} \left[\frac{v_x(0)}{v_y(0)} - \left(\frac{g}{2v_y^2(0)}\right) y_{\text{hit}}\right]. && (1.40) \end{aligned}$$

So one solution is that the object is on the ground at $y = 0$, but this is where we start (remember that we chose $y(0) = 0$). So the interesting solution is found by dividing through by y_{hit},

$$\begin{aligned} 0 &= y_{\text{hit}} \left[\frac{v_x(0)}{v_y(0)} - \left(\frac{g}{2v_y^2(0)}\right) y_{\text{hit}}\right] \\ &= \frac{v_x(0)}{v_y(0)} - \left(\frac{g}{2v_y^2(0)}\right) y_{\text{hit}} && (1.41) \\ y_{\text{hit}} &= \frac{2v_x(0)v_y(0)}{g}. && (1.42) \end{aligned}$$

This is the answer, but it's a little messy, so we'll see if we can simplify.

We see that that, from Fig 1.4, $v_x(0) = v(0)\sin\theta$, where $v(0)$ is the initial speed of the object and θ is the angle that its initial velocity makes with the ground; $\theta = \pi/2$ corresponds to shooting the object straight up and $\theta = 0$ corresponds to skimming along the ground. Similarly $v_y(0) = v(0)\cos\theta$, so that the particle hits the ground at

$$y = \frac{2v_x(0)v_y(0)}{g} = \frac{2v^2(0)\sin\theta\cos\theta}{g}. \tag{1.43}$$

But you may recall that $\sin(2\theta) = 2\sin\theta\cos\theta$, so we have

$$y = \frac{v^2(0)}{g}\sin(2\theta), \tag{1.44}$$

which is a nice, compact result.

Perhaps you have seen Eq (1.44) before, in your high school course. What is important here is to emphasize that this, like all the other formulae of mechanics, are *derivable* from Newton's laws. If we had to remember a different formula for each different situation, it wouldn't really be much of a science. The great achievement of our scientific culture is to have a small set of principles from which everything can be worked out.

Problem 6: Use Eq (1.38) to find the maximum height that the object reaches along its trajectory. Recall that to find the maximum of a function you find the place where the derivative is zero. Notice that in this case you are looking for the maximum value of x viewed as function of y, opposite the usual conventions in textbooks. You should be able to do the same calculation directly from Eq (1.32). Show that you get the same answer.

Drag forces

When you move your arm through the water you feel a force opposing the motion. Part of this force is the inertia of the water that you are moving, but if you go very slowly then the dominant component is the *drag* generated by the viscosity of the water, and this force is proportional to the velocity v. The sign of the force is to oppose motion, so we write $F_{\text{drag}} = -\gamma v$, where γ is called the drag coefficient.

Problem 7: Imagine that we have two flat parallel plates, each of area A, separated by a distance L, and that this space is filled with fluid. If we slide the plates relative to each other slowly, at velocity v (parallel to plates), then we will find that there is a drag force $F_{\rm drag} = -\gamma v$ which acts to resist the motion. Intuitively, the bigger the plates (larger A) and the closer they are together (smaller L) the larger the drag, and in fact over a range of interesting scales one finds experimentally that $\gamma = \eta A/L$, where the proportionality constant η is called the viscosity of the fluid.

(a.) What are the units of viscosity? Instead of expressing your answer in terms of force, length and time, try to express the viscosity as a combination of energy, length and time.

(b.) Viscosity is something we can measure (and "feel") on a macroscopic scale. But the properties of a fluid depend on the properties of the molecules out of which it is made. So if we want to understand why the viscosity of water is $\eta = 0.01$ in the cgs (centimeter–gram–second) system of units, we need to think about the scales of energy, length and time that are relevant for the water molecules. Plausibly relevant energy scales are the energies of the hydrogen bonds between the water molecules (which you can look up), and the thermal energy $k_BT \sim 4\times 10^{-21}\,\text{J}$ at room temperature, which is the average kinetic energy of molecules as they jiggle around in the fluid (more about this later in the semester). The characteristic length is the size of an individual water molecule, or the distance between molecules. What is the range of time scales that combines with these energies and volume to give the observed viscosity? What do you think this time scale means—i. e., what event actually happens on this time scale?

Newton's basic equation

$$m\frac{d^2x(t)}{dt} = F \tag{1.45}$$

can also be written as

$$m\frac{dv(t)}{dt} = F, \tag{1.46}$$

which in this case becomes

$$m\frac{dv(t)}{dt} = -\gamma v(t). \tag{1.47}$$

Here I am being careful to show you that v is a function that depends on time.

It is often said that there are three good ways to solve a differential equation. Best is to ask someone who knows the answer. Next one guesses the form of the solution and checks that it is correct. Finally, there are some more systematic approaches. Let's try one of these, largely so we can build up our intuition and make better guesses next time we need them!

We'd like to solve Eq (1.47) the same way that we did in previous cases, by integrating, but this doesn't work directly—on the right hand side we'd have to integrate $v(t)$ itself, and clearly we don't know how to do this. So we play a little with the equation, doing something which would make a real mathematician cringe:

$$\begin{aligned} m\frac{dv}{dt} &= -\gamma v \\ \frac{dv}{dt} &= -\frac{\gamma}{m}v \qquad (1.48) \\ \frac{dv}{v} &= -\frac{\gamma}{m}dt. \qquad (1.49) \end{aligned}$$

Now we can integrate, since on the left we have v and on the right we have dt, with no mixing. Again we should be careful to do definite integrals from some initial time $t = 0$ up until now (t), during which time the velocity runs from its initial value $v(0)$ to its current value $v(t)$. Notice that we don't actually know the value of $v(t)$; indeed this is what we are trying to find. Nonetheless we can put this value as the endpoint of our integral, and solve at the end:

$$\begin{aligned} \frac{dv}{v} &= -\frac{\gamma}{m}dt \\ \int_{v(0)}^{v(t)} \frac{dv}{v} &= -\frac{\gamma}{m}\int_0^t dt \qquad (1.50) \\ [\ln v]\Big|_{v(0)}^{v(t)} &= -\frac{\gamma}{m}t \qquad (1.51) \\ \ln v(t) - \ln v(0) &= -\frac{\gamma}{m}t \qquad (1.52) \\ \ln\left[\frac{v(t)}{v(0)}\right] &= -\frac{\gamma}{m}t \qquad (1.53) \\ v(t) &= v(0)e^{-\gamma t/m}. \qquad (1.54) \end{aligned}$$

Thus the solution is an *exponential decay.*

Let's be sure we understand the steps leading to Eq (1.54):

Eq (1.50) → (1.51) On the right hand side we just use $\int dt = t$, and on the left we use $\int \frac{dv}{v} = \ln v$, where ln denotes the natural logarithm. Note that this is why natural logarithms are natural!

Eq (1.51) → (1.52) This is just evaluating the indefinite integral at it's endpoints.

Eq (1.52) → (1.53) Now we use $\ln a - \ln b = \ln(a/b)$.

Eq (1.53) → (1.54) Finally, to get rid of the logarithm we exponentiate both sides of the equation. We are using $\ln(e^x) = x$, or equivalently $e^{\ln x} = x$.

Another way of writing our result in Eq (1.54) is

$$v(t) = v(0)e^{-t/\tau}, \tag{1.55}$$

where the time constant $\tau = m/\gamma$. We can see that this is the characteristic time scale in the problem by going back to the original equation:

$$\begin{aligned} m\frac{dv(t)}{dt} &= -\gamma v(t) \\ \frac{m}{\gamma}\frac{dv(t)}{dt} &= -v(t). \end{aligned} \tag{1.56}$$

The combination $\tau = m/\gamma$ must be a time scale in order to balance the units on either side of the equation. This "characteristic time scale" is the only term in the equation that has the units of time, and thus we expect that when we plot the solution we will see all the important variations occurring on this time scale. This is an important idea—we can say on what scale we expect to see things happen even before we solve the equation—and we will come back to it several times in the course.

This is a good place to remind ourselves of a special feature of the exponential function. With $v(t) = v(0)\exp(-t/\tau)$, there is a unique time $t_{1/2}$ such that v is reduced by a factor of two:

$$\begin{aligned} v(t_{1/2}) &\equiv \frac{1}{2}v(0) && (1.57) \\ v(0)\exp(-t_{1/2}/\tau) &= \frac{1}{2}v(0) && (1.58) \\ \exp(-t_{1/2}/\tau) &= 1/2 && (1.59) \\ -t_{1/2}/\tau &= \ln(1/2) && (1.60) \\ t_{1/2}/\tau &= \ln(2) && (1.61) \\ t_{1/2} &= \tau \ln 2. && (1.62) \end{aligned}$$

So as t runs from 0 up to $t_{1/2}$, the velocity goes down by a factor of two. The special feature of the exponential function is that when t advances further, from $t_{1/2}$ to $2 \times t_{1/2}$, the velocity goes down by another factor of two. Thus whenever a time $t_{1/2}$ elapses, the velocity falls to half its value. For this reason we can call $t_{1/2}$ the *half life*: this is the time for the velocity to fall by half, no matter what velocity we start with. More generally, if we look at the evolution from time t to $t + T$, it "looks the same" no matter what point in time t we start with, as long as we rescale the initial value of the function—the change over a window of time T depends on duration of the window (T), not on *when* we look (t). This is illustrated in Fig 1.5.

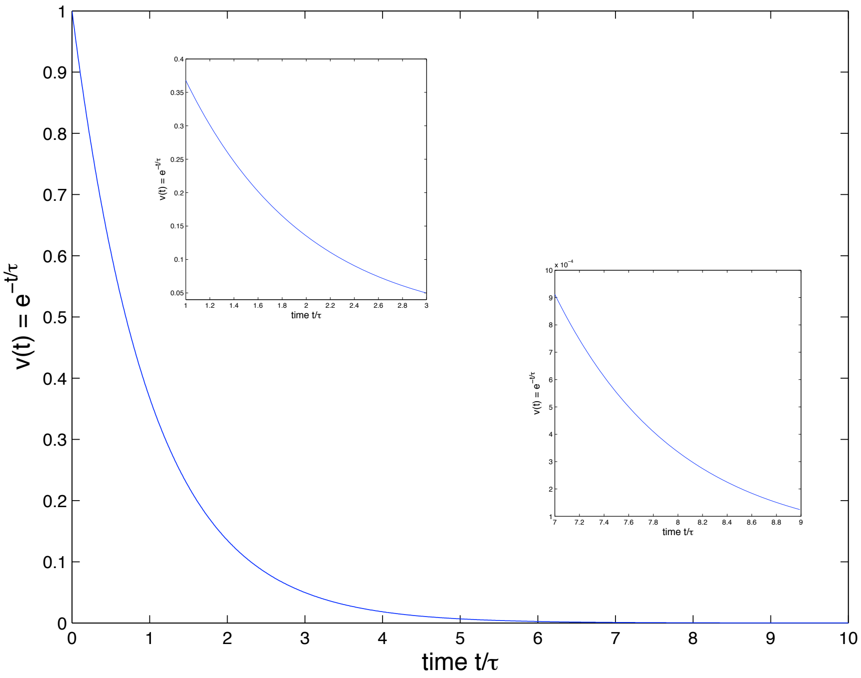


Figure 1.5: Exponential decay, as in Eq (1.55) with $v(0) = 1$. In the insets we focus on two windows of time that have a duration of $T = 2\tau$, starting at different moments. You see that, once we set the scale on the y–axis correctly, the plots look the same.

Problem 8: Consider the motion of a particle subject to a drag force, as in the experiments you are doing in the lab. In the absence of any other forces (including, for the moment, gravity), Newton's equation $F = ma$ can be written as

$$M\frac{dv}{dt} = -\gamma v, \tag{1.63}$$

where M is the mass of the particle and γ is the drag coefficient; we assume that the velocities are small, so the drag force is proportional to the velocity. For a spherical particle of radius r in a fluid of viscosity η, we have the Stokes' formula, $\gamma = 6\pi\eta r$. Assume that the particle also has a mass density of ρ. As shown above, the solution to Eq (3.50) is an exponential decay: $v(t) = v(0)\exp(-t/\tau)$, where the time constant τ determined by all the other parameters in the problem. Be sure that you understand this before doing the rest of this problem!

(a.) Write the time constant τ in terms of M and γ. How does τ scale with the radius of the particle?

(b.) Suppose that the density ρ is close to that of water, and that the relevant viscosity is also that of water. What value (in seconds) do you predict for the time constant τ when the particle has a radius $r \sim 1\,\text{cm}$? What about $r \sim 1\,\text{mm}$ or $r \sim 10\,\mu\text{m}$? Be careful about units!

(c.) A bacterium like *E coli* is approximately a sphere with radius $r = 1\,\mu\text{m}$. Will you ever see the bacterium moving in a straight line because of its inertia?

(d.) What is the relationship between the position $x(t)$ and the velocity $v(t)$? Given that $v(t) = v(0)e^{-t/\tau}$, find a formula for $x(t)$ and sketch the result. Label clearly the major features of your sketch. What happens at long times, $t \gg \tau$?

(e.) *E coli* can swim at a speed of $\sim 20\,\mu\text{m/s}$. Imagine that the motors which drive the swimming suddenly stop at time $t = 0$. Now there are no forces other than drag, but the bacterium is still moving at velocity $v(0) = 20\,\mu\text{m/s}$. How far will the bacterium move before it finally comes to rest?

Problem 9: Let's try to use these same ideas to describe the motion of a person through a swimming pool. Once again the fluid is water, and the density of the "object" is also close to that of water. When a person curls up into a ball, they have a radius of about 50 cm (a meter in diameter). If a person starts moving at speed v_0 through a swimming pool while in this position, then by analogy with the previous problem, what is your prediction about how long it will take for their velocity to fall from v_0 down to $v_0/2$? Does this make sense given your own experience in the water? If not, what do you think has gone wrong? We know that none of you are spherical. You'll have to decide if this is a key issue, or if these calculations are wrong even for the case of the spherical student.

A very different sort of drag arises when objects move more rapidly. Although this isn't the same sort of rigorously justifiable approximation as $F_{\text{drag}} = -\gamma v$, one often finds that drag forces are roughly proportional to the square of the velocity at higher velocities. One then has to be careful about the sign of the force; if the velocity is positive then the force is negative, opposing the motion, so we'll write $F_{\text{drag}} = -cv^2$. Then $F = ma$ becomes

$$m\frac{dv(t)}{dt} = -cv^2(t). \tag{1.64}$$

We proceed as before to integrate the equation:

$$\begin{aligned}
m\frac{dv}{dt} &= -cv^2 \\
\frac{dv}{dt} &= -\left(\frac{c}{m}\right)v^2 && (1.65) \\
\frac{dv}{v^2} &= -\left(\frac{c}{m}\right)dt && (1.66) \\
\int_{v(0)}^{v(t)} \frac{dv}{v^2} &= -\left(\frac{c}{m}\right)\int_0^t dt && (1.67) \\
\left[-\frac{1}{v}\right]\Bigg|_{v(0)}^{v(t)} &= -\left(\frac{c}{m}\right)t && (1.68) \\
-\frac{1}{v(t)} + \frac{1}{v(0)} &= -\left(\frac{c}{m}\right)t && (1.69) \\
\frac{1}{v(0)} + \left(\frac{c}{m}\right)t &= \frac{1}{v(t)} && (1.70) \\
v(t) &= \frac{1}{\frac{1}{v(0)} + \left(\frac{c}{m}\right)t} && (1.71) \\
&= \frac{v(0)}{1 + [cv(0)/m]t}. && (1.72)
\end{aligned}$$

It is convenient to write this as

$$v(t) = \frac{v(0)}{1 + t/t_c}, \tag{1.73}$$

where $t_c = m/[cv(0)]$ is the time at which the velocity has fallen to half of its initial value. Notice that we don't really have a half life in the way that we do for the exponential decay: the velocity falls by a factor of two ($v(0) \rightarrow v(0)/2$) after a time t_c, but if we wait until $t = 2 \times t_c$, the velocity doesn't fall by another factor of two; in fact $v(t = 2t_c) = v(0)/3$, not $v(0)/4$.

Problem 10: Go through the derivation from Eq (1.64) to (1.73) and explain what happens at each step. The strategy for solving the equation is the same as before, but the details are different.

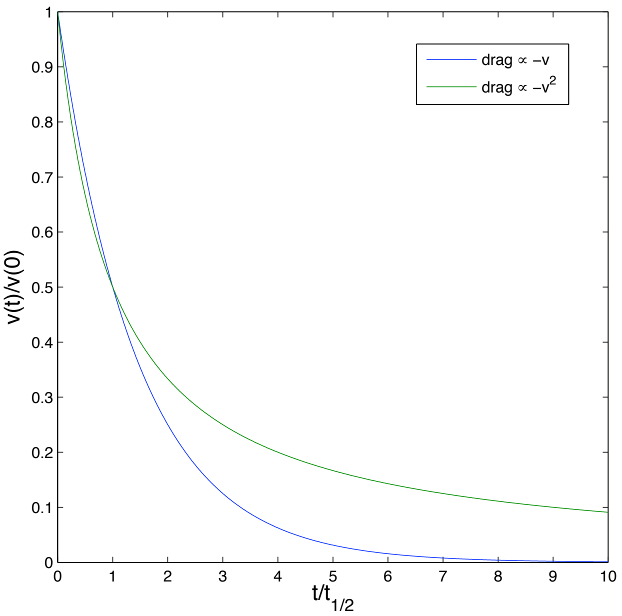


Figure 1.6: Time dependence of velocity for particles experiencing fluid drag. When the drag force is proportional to velocity, the decay is exponential, $v(t) = v(0)\exp(-t/\tau)$, as in Eq (1.55), where $t_{1/2} = \tau \ln 2$. When the drag force is proportional to velocity squared, the decay is asymptotically $\propto 1/t$, as in Eq (1.73).

Figure 1.6 shows the solutions for both $F_{\rm drag} = \gamma v$ and $F_{\rm drag} = -cv^2$, with parameters chosen so that the time to reach half of the initial velocity is the same in both cases. Notice that the behavior at small times is quite similar, but that real differences appear at long times.

It's worth playing with these results, and seeing how the two cases differ, because the same equations arise in thinking about different chemical kinetic schemes, as we'll see in the next section. One interesting point to think about: If we look at the case where $F_{\rm drag} = -cv^2$, then at long times

$$v(t) = \frac{v(0)}{1 + [cv(0)/m]t} \rightarrow \frac{v(0)}{[cv(0)/m]t} = \frac{m}{ct}. \tag{1.74}$$

Thus, after a while ($t \gg t_{1/2}$), the velocity still is decaying with time but the actual value doesn't depend any more on the velocity that we started with! [An improved version of Fig 1.6 would make this last point clearer; maybe you can generate such a figure for yourself.]

One last point: when do we expect to see the drag be linear, and when do we expect it will go as the square of the velocity? This is a great question, and you'll be addressing it in the lab, so we'll leave it for now.

This problem is about an object falling under the influence of gravity, and hence fits with the text a few paragraphs back. It is, however, a bit more open ended than the previous problems, so we place it here at the end of our introduction to $F = ma$.

Problem 11: A simple model of shooting a basketball is that the ball moves through the air influenced only by gravity, so we neglect air resistance. Let's also simplify and not worry about the rotation of the ball, so the dynamics is described just by its position as a function of time. Choose coordinates so the basket is at position $x = 0$ and at a height $y = h$ above the floor (in fact $h = 10\,\mathrm{ft}$, but it's best in these problems not to plug in numbers until the end). When a player located at $x = L$ shoots the ball, it leaves his or her hand at a speed v and at an angle θ measured from the floor (i.e., $\theta = \pi/2$ would be shooting straight up, $\theta = 0$ would correspond to throwing the ball horizontally, parallel to the floor). Assume that the shooter is standing still, and the release of the ball happens at some initial height $y = h_0$ above the floor (in practice h_0 is somewhere between 5 and 7 ft, depending on who's playing).

(a.) Draw a diagram that represents everything you know about the problem, labeling things with all the right symbols. Notice that we are treating this as a problem in two dimensions, whereas of course the real problem is three dimensional.

(b.) What is the equation for the trajectory of the ball with as a function of time after the player releases it? Write your answer as $x(t)$ and $y(t)$, with $t = 0$ the moment of release.

(c.) A perfect shot must arrive at the point $x = 0$, $y = h$ at some time. Presumably the ball also has to traveling downward at this time. Express these conditions as equations that constrain the trajetcory $\{x(t), y(t)\}$, and solve to find allowed values of the speed v and angle θ.

(d.) Saying that the ball must be traveling downward might not be enough. In fact the ball has radius $r = 4.5''$ and the basket has radius $R = 9''$. Continuing with the assumption that we want the ball to pass perfectly through the center of the basket (that is, $x = 0$, $y = h$), what is the real condition on the trajectory?

(e.) The fact that the basket is bigger than the ball means that you don't have to have x exactly equal to zero when $y = h$. To keep things simple let's assume that the shot still will go so long as we get within some critical distance $|x| < x_c$ at the moment when $y = h$. Given what you know so far, what is a plausible value of x_c? Turn this condition on the end of the trajectory into a range of allowed values for v and θ. With typical values for L (think about what these are, or go out to a basketball court and measure!), how accurately does someone need to control v and θ in order to make the shot?

(f.) What we have done here is oversimplified. You are invited to see how far you can go in making a more realistic calculation.[4] Some things to think about are the third dimension (e.g., how accurately does the trajectory need to be "pointed" toward the

---

[4] You might reasonably ask why we care. The fact that people (well, some people, at least) can make these shots with high probability from many different distances is telling us something about ability of the brain to deliver precise motor commands to our

basket?), and a more careful treatment of the ball going through the hoop so that you can state more precisely the condition for making the shot. If you were really ambitious you could think about shots that bounce off the backboard, but that's probably too much for now!

1.2 Chemical reactions: a dynamic perspective

Chemical reactions are processes that involve the transformation of one set of molecules into another and drive many of the interesting phenomena we observe around us. Research in biochemistry over the past century has successfully linked many traits observed in cells and larger organisms with the underlying chemical activities of specific biological molecules. One of the most astounding discoveries in this field was the realization that all living organisms are surprisingly similar on a biochemical level. While the biological world is truly diverse in many ways, many of the molecular players are identical in their size, shape and function across species that are separated from one another by billions of years of evolution.

Chemical kinetics, or reaction kinetics, is the study of the rates of chemical reactions. In this section, we will create a mathematical framework for discussing chemical reactions and find that many of the same differential equations we've already derived come up in this very different context. Let's begin by thinking about how your muscles use energy during exercise. You may know that muscles convert chemical energy, stored in high-energy bonds in a molecule called adenosine triphostphate (ATP), into mechanical work that you can use to run or lift a weight. You also know that you need to breath to make this happen and if you work your muscles too hard they start to fatigue and become painful (due to the buildup of lactic acid). How can we formulate these ideas more concretely?

Reaction diagrams and differential equations

We'll start by writing down diagrammatic versions of what is going on. During aerobic respiration, glucose in your body is combined with the oxygen

---

muscles, since it is the action of our muscles that determine the initial conditions of the ball leaving the hand of the shooter. Although the mechanisms are biological, the constraints are physical. Exploring the constraints makes precise what the system must do in order to achieve the observed level of performance.

you've breathed in to produce carbon dioxide, water and energy in the form of molecules like ATP. We might write this more completely like this

$$C_6H_{12}O_6 + 6O_2 \rightarrow 6CO_2 + 6H_2O$$

Sprinters don't use very much oxygen during a 10 second race. Instead, their bodies metabolize glucose directly to generate the ATP needed for muscle contraction. During this process, which is called glycolysis, one molecule of glucose is converted to two molecules of pyruvate

$$C_6H_{12}O_6 \rightarrow 2CH_3COCOO^-$$

You may have spent some time learning about these reactions and perhaps balancing the number of each kind of atom on each side of a reaction formula. But, what should we make of these formulas? Often, they represent a shorthand for keeping track of the start and end points, the reactants and products, of a reaction. For example, the glycolysis reaction above has been greatly simplified. The entire reaction is really made of many, many sub-reactions, consuming energy from two ATP molecules, but generating four new ATP molecules in the process as shown in Figure 1.7. Other times, the diagram really describes the *mechanism* of the reaction and includes all of the observable intermediate compounds (the letters) and all of the different pathways (the arrows) that can happen. It this case that we will focus on for now.

Consider the following two reactions

$$\begin{aligned} \mathrm{A} &\rightarrow \mathrm{B} \\ \mathrm{A} + \mathrm{B} &\rightarrow \mathrm{C} \end{aligned}$$

If we are to take these seriously, the first reaction describes the conversion of A into B in a *first order* reaction. By first order reaction, we mean that each molecule of type "A" makes an independent decision about whether to complete the reaction and convert to a B–molecule in any given instant in time. In particular, the probability that an A–molecule will become a B–molecule does not depend on encounters with any other molecules. If this is the case, then the number of B–molecules which are created must be proportional to the number of A molecules that are available to react. In chemistry, we usually talk not about the number of molecules, but about their concentrations (i.e. the number per volume). If we write the concentration of species i as C_i, then for our simple first order reaction we have

$$\frac{dC_B}{dt} = kC_A, \tag{1.75}$$

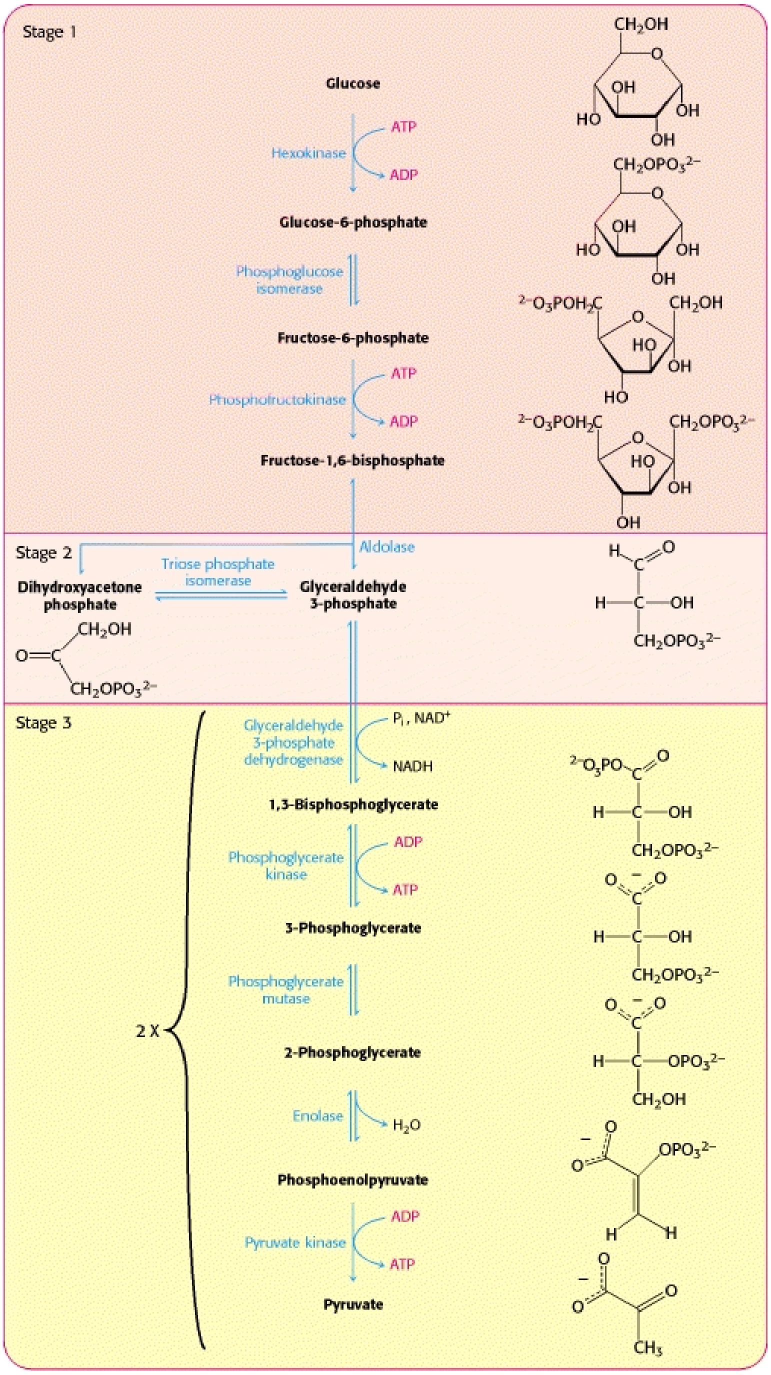


Figure 1.7: The three stages of the glycolysis pathway. From JM Berg, JL Tymocsko & L Stryer, *Biochemistry* (WH Freeman, San Francisco, 2006).

where k is the *first order rate constant*. Note that sometimes one writes $[A]$ to denote the concentration of A. It is important to get used to different notations, as long as they are used consistently within each argument! C_A and C_B have the same units, so in order for Eq (1.75) to make sense, k has to have units of 1/time, conventionally 1/s.

If A is turning into B, then each molecule of B which appears must correspond to a molecule of A which disappeared. Thus we have to have

$$\frac{dC_A}{dt} = -kC_A. \tag{1.76}$$

We've seen this equation before, since it is the same as for the velocity of a particle moving through a viscous fluid, assuming that the drag is proportional to velocity. So we know the solution:

$$C_A(t) = C_A(0)e^{-kt}. \tag{1.77}$$

Then we can also solve for C_B:

$$\begin{aligned}
\frac{dC_B}{dt} &= kC_A \\
&= kC_A(0)e^{-kt} && (1.78)\\
\int_0^t dt\,\frac{dC_B}{dt} &= \int_0^t dt\,kC_A(0)e^{-kt} && (1.79)\\
C_B(t) - C_B(0) &= kC_A(0)\int_0^t dt\,e^{-kt} && (1.80)\\
&= kC_A(0)\left[-\frac{1}{k}e^{-kt}\right]\Bigg|_{t=0}^{t} && (1.81)\\
&= kC_A(0)\left[-\frac{1}{k}e^{-kt} + \frac{1}{k}\right] && (1.82)\\
&= C_A(0)[1 - e^{-kt}] && (1.83)\\
C_B(t) &= C_B(0) + C_A(0)[1 - e^{-kt}]. && (1.84)
\end{aligned}$$

So we see that C_A decays exponentially to zero, while C_B rises exponentially to its steady state; as an example see Fig 1.8. One of the great examples of a first order reaction is radioactive decay, and this is why the abundance of unstable isotopes (e.g., ^{14}C, ^{235}U, ...) in a sample decays exponentially, and this will be very important in the next section.

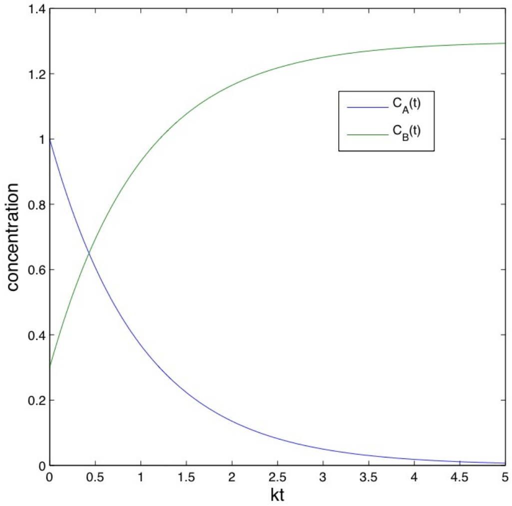


Figure 1.8: Dynamics of the concentrations in a first order reaction $A \to B$.

Problem 12: Just to be sure that you understand first order kinetics ... If the half life of a substance that decays via first order kinetics is $t_{1/2}$, how long do you have to wait until 95% of the initial material has decayed? Explain why this question wouldn't make sense in the case of second order kinetics.

What about the case $\mathrm{A} + \mathrm{B} \to \mathrm{C}$? If we take this literally as a mechanism, we are describing a *second order* reaction, which means that A and B molecules have to find each other in order to make C. The rate at which C molecules are made should thus be proportional to the rate at which these pairwise encounters are happening. What is this rate? If you imagine people milling around at random in a large room, it's clear that the number of times per second that people run into each other depends both on how many people there are and on the size of the room. If you follow one person, the rate at which they run into people should go up if there are more people, and down if the room gets bigger. Plausibly, what matters is the density of people—the number of people divided by the size of the room—which is just like measuring the concentration of molecules.

To obtain the rate of a second order reaction $\mathrm{A} + \mathrm{B} \to \mathrm{C}$, we thus need to count the rate at which A molecules bump into B molecules as they wander around randomly. By analogy with the people milling around the room, if we follow one A molecule, the rate at which it bumps into B molecules will be proportional to the concentration of B molecules. But then the total rate of encounters between A and B will be proportional to the number of A molecules multiplied by the concentration of B, so if we measure the number of encounters per unit volume per second, we'll get an answer proportional to the product of the concentrations of A and B. Thus,

$$\frac{d[C]}{dt} = k_2[A][B]. \tag{1.85}$$

Corresponding the to formation of C is the destruction of both A and B, so we must have

$$\begin{aligned} \frac{d[A]}{dt} &= -k_2[A][B] & (1.86) \\ \frac{d[B]}{dt} &= -k_2[A][B]. & (1.87) \end{aligned}$$

The rate constant k_2 is now a *second order rate constant*, and you can see that it has different units from the first order rate constant k in the equations above; $k_2 \sim 1/(\text{time} \cdot \text{concentration})$, conventionally $1/(\mathrm{M} \cdot \mathrm{s})$.

Perhaps the simplest second order reaction is $\mathrm{A} + \mathrm{A} \rightarrow \mathrm{B}$, for which the relevant equations are

$$\begin{aligned} \frac{d[A]}{dt} &= -k_2[A]^2 & (1.88) \\ \frac{d[B]}{dt} &= k_2[A]^2. & (1.89) \end{aligned}$$

We have seen this equation before, describing the velocity of a particle that experiences drag proportional to velocity squared. Thus we can proceed as we did before:

$$\begin{aligned} \frac{d[A]}{dt} &= -k_2[A]^2 & \\ \frac{d[A]}{[A]^2} &= -k_2 dt & (1.90) \\ \int_{[A]_0}^{[A]_t} \frac{d[A]}{[A]^2} &= k_2 \int_0^t dt & (1.91) \\ -\frac{1}{[A]}\Big|_{[A]_0}^{[A]_t} &= -k_2 t & (1.92) \\ -\frac{1}{[A]_t} + \frac{1}{[A]_0} &= -k_2 t & (1.93) \\ \frac{1}{[A]_0} + k_2 t &= \frac{1}{[A]_t} & (1.94) \\ [A]_t &= \frac{[A]_0}{1 + k_2[A]_0 t}, & (1.95) \end{aligned}$$

where $[A]_t$ is the concentration of A at time t, and in particular $[A]_0$ is the concentration when $t = 0$. Thus the initial concentration does not decay as an exponential, but rather as $\sim 1/t$ at long times; the time for decay to half the initial value is $t_{1/2} = 1/(k_2[A]_0)$ and depends on the initial concentration. Notice that

$$[A]_{t \gg t_{1/2}} \approx \frac{[A]_0}{k_2[A]_0 t} = \frac{1}{k_2 t}, \tag{1.96}$$

so that after a while the concentration is still changing, but the amount of stuff we have left is independent of how much we started with (!).

Problem 13: Check that you understand each of the steps leading to Eq (1.95). As a test of your understanding, consider the (rather unusual) case of a third order reaction, in which three A molecules come together to react irreversibly. This is described by

$$\frac{d[A]}{dt} = -k_3[A]^3. \tag{1.97}$$

What are the units of the third order rate constant k_3? Can you solve this equation?

time t (minutes)	$[A]/[A]_0$	$[B]/[B]_0$
0.25	0.7157	0.7635
0.50	0.7189	0.4305
0.75	0.5562	0.5262
1.00	0.4761	0.6195
1.25	0.4948	0.4876
1.50	0.3096	0.3169
1.75	0.3842	0.3702
2.00	0.2022	0.2764
2.25	0.1872	0.2613
2.50	0.1971	0.2738

Table 1.1: Two kinetics experiments.

Problem 14: Imagine that you do two experiments in chemical kinetics. In one case we watch the decay of concentration is some reactant A, and in the other case the reactant is B. The half lives of both species are about one minute, and perhaps because you are in a hurry you run the reactions out only for 2.5 minutes. You take samples of the concentration every quarter of a minute, and you get the results in Table 1.1. Perhaps the first thing you notice is that the concentrations don't decrease monotonically with time. Presumably this is the result of errors in the measurement.

(a.) Can you decide whether the reactions leading to the decay of A and B are first order or second order? Are A and B decaying in the same way, or are they different?

(b.) Other than making more accurate measurements, how could you extend these experiments to give you a better chance at deciding if the reactions are first or second order?

Problem 15: An important step in the production of sulfuric acid involves the change of sulfur dioxide into sulfur trioxide. Sulfur dioxide, SO_2, can react with oxygen to give sulfur trioxide, SO_3 through the use of vanadium oxide

$$\mathrm{SO_2} + \frac{1}{2}\mathrm{O_2} \xrightarrow{\mathrm{V_2O_5}} \mathrm{SO_3}$$

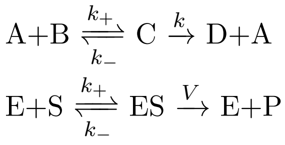
If you do this in the lab, you will find that tripling the sulfur dioxide concentration increases the rate by a factor of about 3. But tripling the sulfur trioxide concentration lowers the reaction rate by a factor of about 1.7. You will also find that the rate is insensitive to the oxygen concentration as long as you have enough of it.

(a.) Write down the kinetic differential equation for this reaction. What are the units of the rate constant?

(b.) If $[SO_2]$ is increased by a factor of 2 and $[SO_3]$ is increased by a factor of 5, by how much will the overall reaction change?

An important point about all this is that when we draw a more complex reaction mechanism, each and every arrow corresponds to a term in the differential equation, and the sign of the term depends on the direction of the arrow. Consider, for example, the reactions shown at the top of Fig 1.9. Really this is a scheme in which B is converted into D, and the A molecules participate but are not consumed: the A molecules are catalysts. Notice that there are three separate reactions, one for each arrow: $A + B \to C$, which occurs with a second order rate constant k_+, $C \to A + B$, which occurs with first order rate k_-, and $C \to D + A$, with first order rate k. We write k_+ and k_- because these are forward and reverse processes.

Now we have to write out the differential equations, using the rule that each reaction or arrow generates its corresponding term. Probably it's easiest to start with the equation for $[C]$, since all three reactions contribute. We see the arrow coming "in" to C from the left, which corresponds to the concentration of C changing at a rate $k_+[A][B]$. There is a second arrow at the left, which corresponds to the concentration of C changing at a rate $-k_-[C]$, where the negative sign is because the arrow points "out" and describes the destruction of C molecules. Finally, there is an arrow point out



$$\mathrm{A+B} \underset{k_-}{\overset{k_+}{\rightleftharpoons}} \mathrm{C} \xrightarrow{k} \mathrm{D+A}$$

$$\mathrm{E+S} \underset{k_-}{\overset{k_+}{\rightleftharpoons}} \mathrm{ES} \xrightarrow{V} \mathrm{E+P}$$

Figure 1.9: At the top, a reaction scheme for the conversion of B into D, using A as a catalyst. At the bottom, this scheme is written to make better connections with the idea of catalysis by an enzyme: E is the enzyme, S is the 'substrate' that gets converted into the product P, and ES is a complex of the enzyme and substrate bound to one another. The rate constants $k_\pm$ have the same notation, but we write the rate for $ES \rightarrow E + P$ as V, since it's the 'velocity' of the enzyme.

to the right, which corresponds to the concentration of C changing at a rate $-k[C]$. Putting all of these terms together, we have

$$\frac{d[C]}{dt} = +k_+[A][B] - k_-[C] - k[C]. \tag{1.98}$$

For $[B]$, only the k_+ and k_- processes contribute:

$$\frac{d[B]}{dt} = -k_+[A][B] + k_-[C]. \tag{1.99}$$

Finally, for $[A]$, all three reactions contribute, but with the opposite signs from Eq (1.98):

$$\frac{d[A]}{dt} = -k_+[A][B] + k_-[C] + k[C]. \tag{1.100}$$

The important point here is not to solve these equations (yet), but rather to be sure that you understand how to go from the pictures with arrows describing the reactions down to the equations that describe quantitatively the dynamics of the concentrations.

Catalysis

A catalyst is a substance that takes part in a chemical reaction and speeds up the rate but undergoes no permanent chemical change itself. The enhancement of the reaction rate can come from speeding up existing pathways between the reactants and products or, more commonly, providing completely new pathways by which a reaction can occur. We won't be able to discuss the energetics of how a catalyst works until later in the semester, but for now we can examine the dynamics of these economically important compounds. Industrial chemistry devotes great effort to finding catalysts to accelerate particular desired reactions without increasing the generation of undesired products.

One example of a complex catalyst that you've all encountered is the solid catalyst used to reduce the emission of pollutants such as unburned hydrocarbons, carbon monoxide, and nitrogen oxides in the exhaust of a car engine. A catalytic converter is designed to simultaneously *oxidize* hydrocarbons and carbon monoxide through the reactions

$$\mathrm{CO, C_xH_y, O_2} \xrightarrow{\text{Catalyst}} \mathrm{CO_2, H_2O}$$

and *reduce* nitrogen oxides through the reactions

$$\mathrm{NO, NO_2} \xrightarrow{\text{Catalyst}} \mathrm{N_2, O_2}$$

Clearly, the best catalyst for the reduction reactions may not be the best for the oxidation reactions, so two catalysts are usually combined. For performance reasons, expensive noble metals, usually platinum as an oxidation catalyst and rhodium as a reduction catalyst, are deposited on a fine alumina mesh which gives a large interaction surface area. Because lead blocks these catalysts, you have to use unleaded gasoline in your (modern) car. The use of expensive materials makes your catalytic converter one of the most valuable objects in your car and there are numerous examples of people stealing converters off of cars to sell on the black market.

In the bottom of Fig 1.9 ,we have rewritten the catalysis reaction to make clear that it describes an enzyme 'E' which converts 'substrates' S into 'products' P. In fact this is one of the standard schemes for describing biochemical reactions, and it's called Michaelis–Menten kinetics. To make contact with the standard discussion, let's call the concentration of substrates $[S]$, the concentration of products $[P]$, and so on. Then the kinetic equations become

$$\frac{d[S]}{dt} = -k_+[S][E] + k_-[ES] \quad (1.101)$$

$$\frac{d[ES]}{dt} = k_+[S][E] - (k_- + V)[ES] \quad (1.102)$$

$$\frac{d[P]}{dt} = V[ES] \quad (1.103)$$

$$\frac{d[E]}{dt} = -k_+[S][E] + (k_- + V)[ES] \quad (1.104)$$

You should notice that Eq's (1.102) and (1.104) can be combined to tell us that

$$\frac{d([ES] + [E])}{dt} = 0, \quad (1.105)$$

or equivalently that $[ES] + [E] = [E]_0$, the total enzyme concentration. Solving all these equations is hard, but there is an approximation in which everything simplifies which was first introduced by Briggs and Haldane in 1924.

Suppose that there is a lot of the substrate, but relatively little enzyme. Then the high concentration of the substrate means that the binding of the substrate to the enzyme will be fast. Although this isn't completely obvious, one consequence is that the concentration of the enzyme–substrate complex ES will come very quickly to a steady state; in particular this steady state will be reached before the substrate concentration has a chance to change very much. But we can find this steady state just by setting $d[ES]/dt = 0$ in Eq (1.102):

$$\begin{aligned} 0 = \frac{d[ES]}{dt} &= k_+[S][E] - (k_- + V)[ES] && (1.106) \\ \Rightarrow 0 &= k_+[S][E] - (k_- + V)[ES] && (1.107) \\ k_+[S][E] &= (k_- + V)[ES]. && (1.108) \end{aligned}$$

Now we use the constancy of the total enzyme concentration, $[ES] + [E] = [E]_0$, to write $[E] = [E]_0 - [ES]$, and substitute to solve for $[ES]$:

$$\begin{aligned} k_+[S][E] &= (k_- + V)[ES] \\ k_+[S]([E]_0 - [ES]) &= (k_- + V)[ES] && (1.109) \\ k_+[S][E]_0 - k_+[S][ES] &= (k_- + V)[ES] && (1.110) \\ k_+[S][E]_0 &= (k_- + V)[ES] + k_+[S][ES] && (1.111) \\ &= (k_- + V + k_+[S])[ES] && (1.112) \\ \frac{k_+[S][E]_0}{k_- + V + k_+[S]} &= [ES]. && (1.113) \end{aligned}$$

The reason it is so useful to solve for $[ES]$ is that, from Eq (1.103), the rate at which product is formed is just $V[ES]$, so we find

$$\frac{d[P]}{dt} = V[E]_0 \frac{k_+[S]}{k_- + V + k_+[S]}, \tag{1.114}$$

or

$$\frac{d[P]}{dt} = V[E]_0 \frac{[S]}{[S] + K_m}, \tag{1.115}$$

where $K_m = (k_- + V)/k_+$ is sometimes called the Michaelis constant.

What is this formula telling us? To begin, the rate at which we make product is proportional to the concentration of enzymes. Although we have

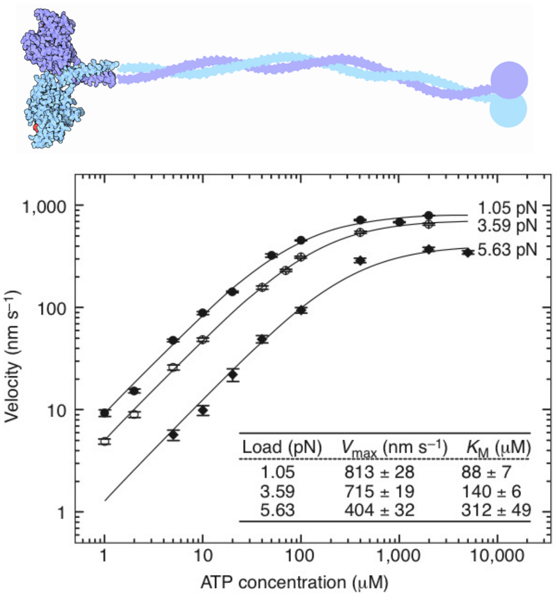


Figure 1.10: The translational velocity of a single kinesin "motor" walking along a microtubule as a function of ATP concentration under different forces. For each force, the force–velocity relationship follows the Michaelis-Menten formula, but the specific values of K_M and V change with force. Note that because the velocity is measured for a single enzyme, there is no enzyme concentration, E_0, to worry about. From K Visscher, MJ Schnitzer & SM Block, Single kinesin molecules studied with a molecular force clamp. *Nature* **400,** 184–189 (1999).

written equations for the macroscopic concentration of molecules, we can think of this in terms of what individual molecules are doing: each enzyme molecule can turn substrate into product at some rate, and the total rate is then this 'single molecule' rate multiplied by the total number of enzyme molecules. In addition, Eq (1.115) tells us that if the substrate concentration is really low ($[S] \ll K_m$), then the rate at which catalysis happens is proportional to how much substrate we have; on the other hand once the substrate concentration is large enough ($[S] \gg K_m$), finding substrate molecules is not the problem and the rate of catalysis is limited by the properties of the enzyme itself (V).

Equation (1.115) is the main result of Michaelis–Menten kinetics, and it is widely used to describe real enzymes as they catalyze all sorts of reactions inside cells. One beautiful demonstration of this type of kinetics can be seen using the enzyme kinesin, a "molecular motor" that catalyzes the hydrolysis of ATP ($\mathrm{ATP} \rightarrow \mathrm{ADP} + \mathrm{P_i}$) in order to walk with two feet along a long filament called a microtubule in your cells (Fig. 1.10). Every time a kinesin hydrolyzes one ATP it takes an 8–nm step along the microtubule. At low ATP concentrations, the speed of a walking kinesin is slow and proportional to the ATP concentration. As you raise the ATP concentration, the speed increases but eventually saturates to about 100 steps per second.

The two main parameters in the Michaelis-Menten equation, $\mathrm{K_M}$ and V, are properties of the enzyme itself. For most enzymes in your body, $\mathrm{K_M}$ has values in the range of 10^{-1} to 10^{-7}M. The larger this value, the more substrate is needed to push the reaction into the saturated regime. The effect of different $\mathrm{K_M}$ values on human physiology can be seen in examining the sensitivity of some people to the effects of digesting ethanol. As you may know, some people experience a redness of the face and rapid heart rate when they ingest alcohol, which is caused by an excess of acetaldehyde in the blood. The break down of ethanol in your body takes place in several steps in the liver. Ethanol is first converted into acetaldehyde by an enzyme called Alcohol dehydrogenase

$$\mathrm{CH_3CH_2OH + NAD^+ \xrightleftharpoons{\text{Alchohol dehydrogenase}} CH_3CHO + H^+ + NADH}$$

The acetaldehyde is then broken down into acetate by the enzyme Aldehyde dehydrogenase

$$\mathrm{CH_3CHO + NAD^+ + H_2O \xrightleftharpoons{\text{Aldehyde dehydrogenase}} CH_3COO^- + NADH + 2H^+}$$

Most people have two active forms of this second enzyme, a low and a high $\mathrm{K_M}$ form. In people with hightened sensitivity to ethanol, the low $\mathrm{K_M}$ form contains a single amino acid substitution and is unable to process the acetaldehyde. Therefore, only the high $\mathrm{K_M}$ is active and it is only able to work quickly when the concentration of the acetaldehyde substrate is high. As a consequence, less of the chemical is converted to acetate and more is released into the blood which induces the physiological response. All because a single enzyme contains a single amino acid substitution!

Problem 16: The enzyme lysozyme helps to break down complex molecules built out of sugars. As a first step, these molecules (which we will call S) must bind to the enzyme. In the simplest model, this binding occurs in one step, a second order reaction between the enzyme E and the substrate S to form the complex ES:

$$E + S \overset{k_+}{\to} ES, \tag{1.116}$$

where k_+ is the second order rate constant. The binding is reversible, so there is also a first order process whereby the complex decays into its component parts:

$$ES \overset{k_-}{\to} E + S, \tag{1.117}$$

where k_- is a first order rate constant. Let's assume that everything else which happens is slow, so we can analyze just this binding/unbinding reaction.

(a.) Write out the differential equations that describe the concentrations of $[S]$, $[E]$ and $[ES]$. Remember that there are contributions from both reactions (1.116) and (1.117).

(b.) Use the differential equations you have written to show that if we start with an initial concentration of enzyme $[E]_0$ and zero concentration of the complex ($[ES]_0 = 0$), then there is a conservation law: $[E] + [ES] = [E]_0$ at all times.

(c.) Assume that the initial concentration of substrate $[S]_0$ is in vast excess, so that we can always approximate $[S] \approx [S]_0$. Show that there is a steady state at which the concentration of the complex is no longer changing, and that at this steady state

$$[ES]_{\rm ss} = [E]_0 \cdot \frac{[S]}{[S] + K}, \tag{1.118}$$

where K is a constant. How is K related to the rate constants k_+ and k_-?

(d.) When the substrate is (N–acetylglucosamine)$_2$, experiments near neutral pH and at body temperature show that the rate constants are $k_+ = 4 \times 10^7\,{\rm M^{-1}s^{-1}}$ and $k_- = 1\times10^5\,{\rm s^{-1}}$. What is the value of the constant K [in Eq (1.118)] for this substrate? At a substrate concentration of $[S] = 1\,{\rm mM}$, what fraction of the initial enzyme concentration will be in the the complex $[ES]$ once we reach steady state?

(e.) Show that the concentration of the complex $[ES]$ approaches its steady state exponentially: $[ES](t) = [ES]_{\rm ss}[1 - \exp(-t/\tau)]$. Remember that we start with $[ES]_0 = 0$. How is the time constant τ related to the rate constants k_+ and k_- and to the substrate concentration $[S]$? For (N–acetylglucosamine)$_2$, what is the *longest* time τ that we will find for the approach to steady state?

Problem 17: The data from Figure 1.10 were taken using a sophisticated Optical Trap[5] that can both track the motion of a single enzyme at very high resolution and apply a physical force to the enzyme. As you can see from the figure, pulling backwards on the kinesin motor changes both the maximum speed V and the Michaelis constant K_M. If only one of the rates in Fig. 1.9 were to depend on force, could you explain the data shown in the table? Explain your answer.

Problem 18: Under physiological conditions, most enzymes are sub–saturated with $[{\rm S}]/{\rm K_M}$ between 0.01 and 1.

(a.) At what rate does the enzyme go under these circumstances? Show that for $[S] \ll K_M$

$$\frac{dP}{dt} \approx \frac{V}{K_M}[E]_0[S] \tag{1.119}$$

(b.) In some sense, the ratio V/K_M is a measure of the efficiency of catalysis as it takes into account both the rate of substrate binding, via K_M, and the rate of catalysis, through V. It is worth asking how "efficient" an enzyme can be. Show that $(V/K_M) < k_+$ must be true.

(c.) Thinking about what the rate k_+ describes, what is the physical nature behind this limit on the enzymatic rate?

Another interesting example is a sequence or cascade of reactions, as schematized in Fig 1.11. Here we imagine that there is a molecule A which

---

[5] For more information on this technology, see `http://en.wikipedia.org/wiki/Optical_tweezers`

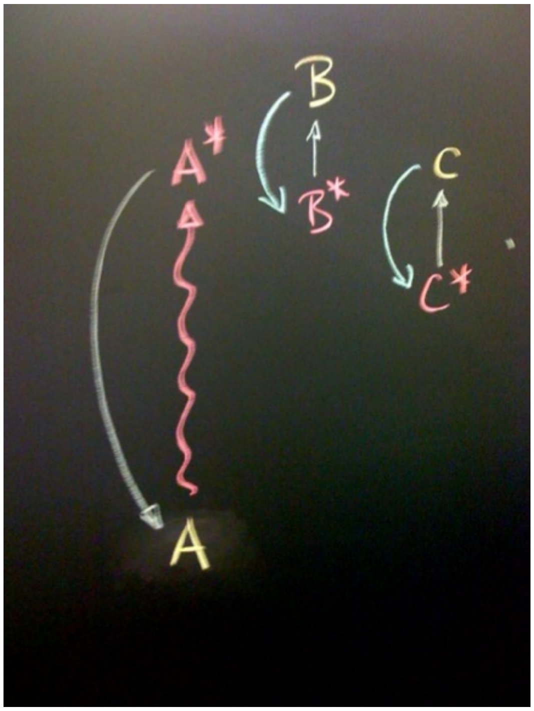


Figure 1.11: A cascade of enzymatic reactions.

can be stimulated by some signal to go into an activated state A^*. Once in this activated state, it can act as a catalyst, converting B molecules into their activated state B^*. The active B^* molecules act as a catalyst for C, and so on. This sort of scheme is quite common in biological systems, and serves as a molecular amplifier—even if we activate just one molecule of A, we can end up with many molecules at the output of such a cascade.

One example that we should keep in mind is happening in the photoreceptor cells of your retina as you read this. In these cells, the A molecules are rhodopsin, and the stimulation is what happens when these molecules absorb light. Once rhodospin is in an active state, it can catalyze the activation of the B molecules, which are called transducin. Transducin is one member of a large family of proteins (called G–proteins) that are involved in many different kinds of signaling and amplification in all cells, not just vision. The C molecules are enzyme called phosphodiesterase, which chew up molecules of cyclic GMP (cGMP, which would be D if we continued our schematic). Again, lots of cellular processes use cyclic nucleotides (cGMP and cAMP) as internal signals or 'second messengers' in cells. In the photoreceptors, cGMP binds to proteins in the cell membrane that open holes in the membrane, and this allows the flow of electrical current; more about this later in the course. These electrical signals get transmitted to other cells in the retina, eventually reaching the cells that form the optic nerve and carry information from the eye to your brain.

How can we describe the dynamics of a cascade such as Fig 1.11? Let's think about the way in which $[B^*]$ changes with time. We have the idea that A^* catalyzes the conversion of B into B^*, so the simplest possibility is that this is a second order process: the rate at which B^* is produced will be proportional both to the amount of A^* and to the number of available B molecules, with a second order rate constant k_2. Presumably there is also a back reaction so that B^* converts back into B at some rate k_-. Then the dynamics are described by

$$\frac{d[B^*]}{dt} = k[A^*][B] - k_-[B^*]. \tag{1.120}$$

There must be something similar for the way in which C^* is formed by the interaction of B^* with C, and for simplicity let's assume that all the rate constants are the same (this doesn't matter for the point we want to make here!):

$$\frac{d[C^*]}{dt} = k[B^*][C] - k_-[C^*]. \tag{1.121}$$

Actually solving these equations isn't so simple. But let's think about what happens at very early times. In Eq (1.120), we can assume that at $t = 0$ we start with none of the activated B^*. The external stimulus (e.g., a flash of light to the retina) comes along and suddenly we have lots of A^*. There's plenty of B around to convert, and so there is an initial rate $k[A^*]_0[B]_0$, which means that the number of activated B molecules will grow

$$[B^*] \approx k[A^*]_0[B]_0 t. \tag{1.122}$$

Now we can substitute this result into Eq (1.121) to find the dynamics of $[C^*]$ at short times, again assuming that we start with plenty of $[C]$ and none of the activated version:

$$\begin{aligned} \frac{d[C^*]}{dt} &\approx k(k[A^*]_0[B]_0 t)[C] = \{k^2[A^*]_0[B]_0[C]_0\}t & (1.123)\\ \Rightarrow [C^*] &\approx \left(\frac{1}{2}k^2[A^*]_0[B]_0[C]_0\right)t^2 & (1.124) \end{aligned}$$

So we see that the initial rise of $[B^*]$ is as the first power of time, the rise of $[C^*]$ is as the second power, and hopefully you can see that if the cascade continued with C^* activating D, then $[D^*]$ would rise as the third power of time, and so on. In general, if we have a cascade with n steps, we expect that the output of the cascade will rise as t^n after we turn on the external stimulus.

Many people had the cascade model in mind for different biological processes long before we knew the identity of any of the molecular components. The idea that we could count the number of stages in the cascade by looking at how the output grows at short times is very elegant, and in Fig 1.12 we see a relatively modern implementation of this idea for the rod photoreceptors in the toad retina. It seems there really are three stages to the cascade!

This same basic idea of counting steps in a cascade has been used in very different situations. As an example, in Fig 1.13, we show the probability that someone is diagnosed with colon cancer as a function of their age. The idea is the same, that there is some cascade of events (mutations, presumably), and the power in the growth vs. time counts the number of stages. It's kind of interesting that if you look only on a linear plot (on the left in Fig 1.13), you might think that there was something specifically bad that happens to people in their 50s that causes a dramatic increase in the rate at which they get cancer. In contrast, the fact that incidence just grows as a power of age suggest that there is nothing special about any particular age, just that as we get older there is more time for things to have accumulated, and there are several things that need to happen in order for cancer to take hold. It's quite amazing it is that these same mathematical ideas describe such different biological processes occurring on completely different time scales (years vs. seconds).

One can do a little more with the cascade model. If we think a little more (or maybe use the equations), we see that the maximum number of $[B^*]$ molecules that will get made depends on their lifetime $\tau = 1/k_-$: there is a competition between A^* activating $B \rightarrow B^*$, and the decay process $B^* \rightarrow B$. This same story happens at every stage, so again the peak number of molecules at the output will be proportional to some power of the lifetime of the activated molecules, and this power again counts the number of stages in the cascade, Thus the cell can adjust its sensitivity—the peak number of output molecules that each activated input A^* can produce—by modulating the lifetimes of the activated states. But if we change this lifetime, we also change the overall time scale of the response. Roughly speaking, the time required for the response to reach its peak is also proportional to τ. So we expect that if a cell adjusts its gain by changing lifetimes, then the gain and time to peak should be related to each other as gain $\propto t^n_{\text{peak}}$, where there are n stages in the cascade; of course this value of n should agree with what

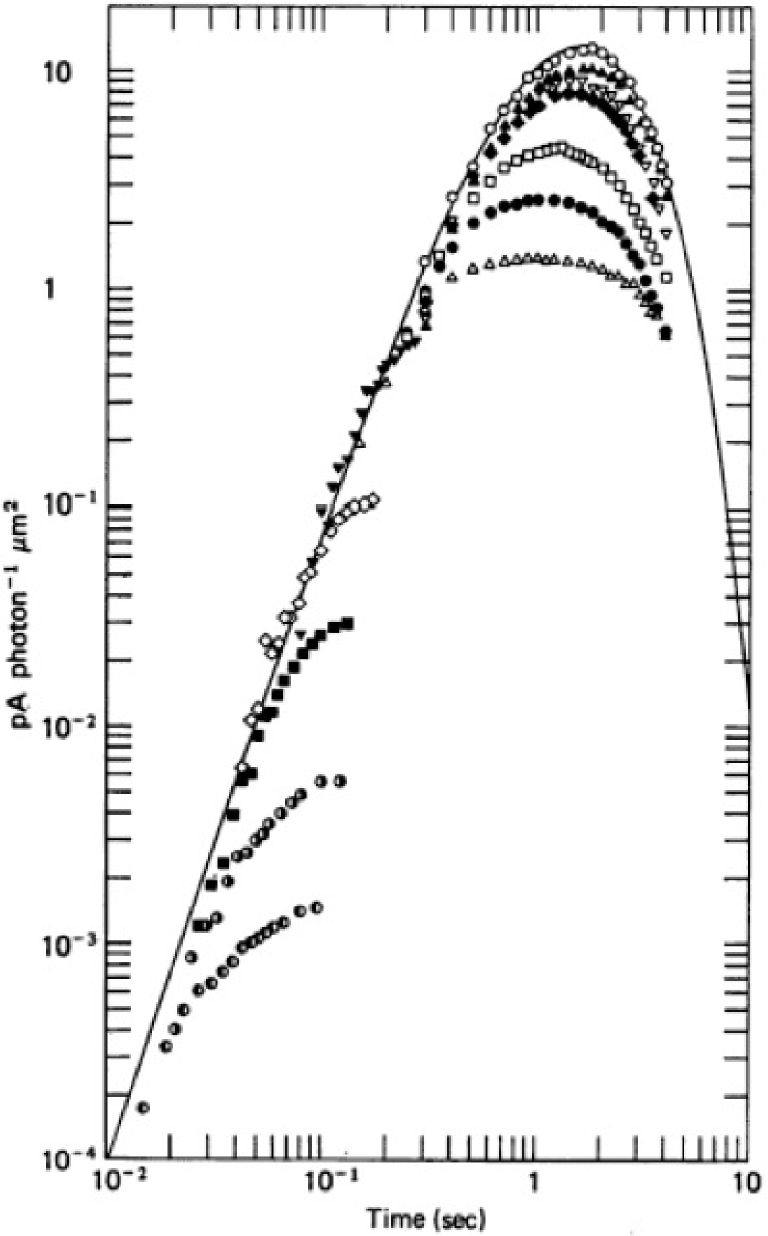


Figure 1.12: Kinetics of the rod photoreceptor response to flashes of light. The data points are obtained by measuring the current that flows across the cell membrane as a function of time after a brief flash of light. Different shape points correspond to brighter or dimmer fshes, and the response is normalize by taking the current (in pA, picoAmps; pico = 10^{-12}) and dividing by the light intensity (in photons per square micron). The lowest intensity flashes give the highest sensitivity, but it's hard to see the response at very early time because it's so small. As you go to brighter flashes you can see the behavior at small times, but then as time goes on the response tends to saturate so what is shown here is just the beginning. Solid line is $r(t) = A\exp(-t/\tau)[1-\exp(-t/\tau)]^3$, which starts out for small t as $r(t) \propto t^3$. From DA Baylor, TD Lamb & K–W Yau, The membrane current of single rod outer segments. *J Physiol* **288,** 589–611 (1979).

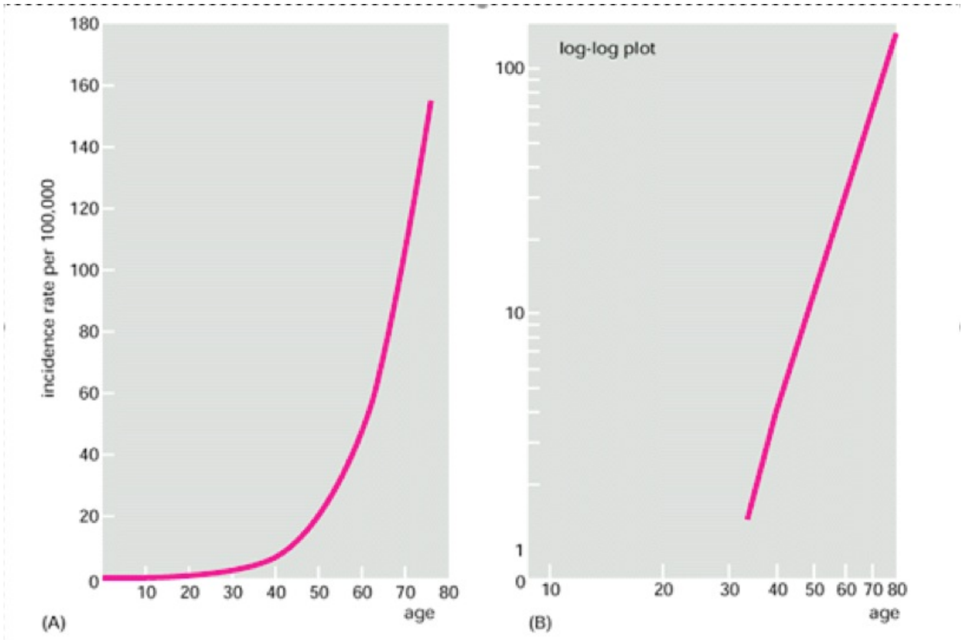


Figure 1.13: Incidence of colon cancer as a function of age. The original data, collected by C Muir et al (1987), refer to women in England and Wales, and are expressed as the number of diagnoses in one year, normalized by the size of the population. At left the data are plotted vs age on a linear scale, and on the right the are replotted on a log–log scale, as in Fig 1.12. What we show here is reproduced from *Molecular Biology of the Cell, 4th Edition*, B Alberts et al (1994). In the next version of these notes we'll go back and look at the original data.

we find by look at the initial rise in the output vs. time. A series of lovely experiments in the 1970s showed that this actually works!

What's nice about this example is that people were using it to think about how your retina adapts to background light intensity long before we had the slightest idea what was really going inside the cells. The fact that simple models could fit the shape of the response, and that these models suggested a simple view of adaptation, was enough to get everyone thinking in the right direction, even if none of the details were quite right the first time through. This is a wonderful reminder of how we should take seriously the predictions of simple models, and how we can be guided to the right picture even by theories that gloss over many details. Importantly, this works just as well inside cells as it does for more traditional physics problems.

1.3 Radioactivity and the age of the solar system

Most of you are familiar with the phenomenon of radioactive decay: Certain elements have *isotopes* in which the nucleus is not stable but rather decays, usually emitting some particle in the process. As an example, we have the "beta decay" of the carbon isotope ^{14}C,

$$^{14}\mathrm{C} \rightarrow {}^{14}\mathrm{N} + e^- + \bar{\nu}_e. \tag{1.125}$$

This means that the carbon nucleus decays into a nitrogen nucleus, giving off an electron (e^-) and a particle you might not know about called an anti–neutrino ($\bar{\nu}_e$); the subscript e means that this particular neutrino is associated with the electron.

To back up a bit, let's recall that most of the carbon around us is ^{12}C. If you look at the periodic table you can see that carbon has six electrons, and since the atom is neutral there must also be six protons in the nucleus; 6 is the "atomic number" of carbon. The "mass number" of 12 comes from these six protons plus six neutrons. The isotope ^{14}C has the same number of electrons and protons—that's what it means to be an isotope!—but two extra neutrons in its nucleus.

Looking again at the periodic table, nitrogen has seven electrons and hence seven protons; ^{14}N thus has seven neutrons. So what is happening in the beta decay of ^{14}C really is

$$6 \text{ protons} + 8 \text{ neutrons} \rightarrow 7 \text{ protons} + 7 \text{ neutrons} + e^- + \bar{\nu}_e, \tag{1.126}$$

or more simply the decay of a neutron (n) into a proton (p^+), an electron and an anti–neutrino,

$$n \rightarrow p^+ + e^- + \bar{\nu}_e. \tag{1.127}$$

If you just have a neutron sitting in free space, this takes about twelve minutes (!). But with all the particles trapped in the nucleus, it can take much longer: more than 5000 years for the decay of ^{14}C.

What you measure when you have a radioactive element is the extra emitted particle, the electron in the case of ^{14}C. So unlike the usual case in chemistry, you don't measure the concentration of each species, you actually measure the transitions from one species to the other. The particles that come out of radioactive decays often have enough energy that you can count the individual particles, so this is like observing chemical reactions one molecule at a time. As we will discuss later in the course, the behavior of individual molecules or individual nuclei is random, so if you watch 1000

^{14}C atoms for $t_{1/2} = 5730$ yr, you won't see exactly 500 decays, but rather some random number which on average is equal to 500. Let's not worry about this randomness for now.

Since every nucleus does its thing on its own, the average number of decays per second (or per year, or per millennium) must be proportional to the number of nuclei that we start with. Since ^{14}C decays but no other nuclei decay into ^{14}C, the dynamics of the concentration of these atoms in a sample is very simple:

$$\frac{d[^{14}\mathrm{C}]_t}{dt} = -\lambda[^{14}\mathrm{C}]_t, \tag{1.128}$$

where λ is the decay rate. By now we know the solution to this equation,

$$[^{14}\mathrm{C}]_t = [^{14}\mathrm{C}]_0 \exp(-\lambda t). \tag{1.129}$$

The concentration falls by half in a time $t_{1/2} = \ln 2/\lambda$, and again this is $t_{1/2} = 5730$ yr for ^{14}C.

You may know that ^{14}C is used to determine the age of fossils and other organic materials. The idea is that as long an organism is alive, it constantly is exchanging carbon with its environment (eating and excreting) and so the isotopic composition of the organism matches that of the atmosphere. Once the organism dies, this exchange stops, and the ^{14}C trapped in the system starts to decay. If we know, for example, that the $^{14}\mathrm{C}/^{12}\mathrm{C}$ ratio was the same in the past as it is today (which is almost true, but hang on for a surprise ...), then if we see less ^{14}C it must be because this isotope has decayed (^{12}C is stable). Since we know the decay rate, the amount of the decay can be translated back into a time, which is the time elapsed since the object "died" and stopped exchanging carbon with the atmosphere. This is the basis of radiocarbon dating.

Because the half life of ^{14}C is about 5000 years, it's a great tool for archaeologists. It's hard, on the other hand, to use ^{14}C to date something more recent. How could we know, for example, if something were 10 or 50 years old? In 10 years there is only a $\sim 10/5000 = 0.002$ decay of the ^{14}C nuclei, so to distinguish things with 10 year accuracy means making measurements to an accuracy of nearly one part in 1000—not so easy. But, in fact, the isotopic composition of the atmosphere is changing rapidly. For a brief period of time in the 1950s and 60s, human beings tested nuclear weapons by exploding them in the atmosphere. This ended with the signing of the nuclear test ban treaty in 1963. The testing produced a significant increase in atmospheric ^{14}C, and since (roughly) 1963 this has been decaying

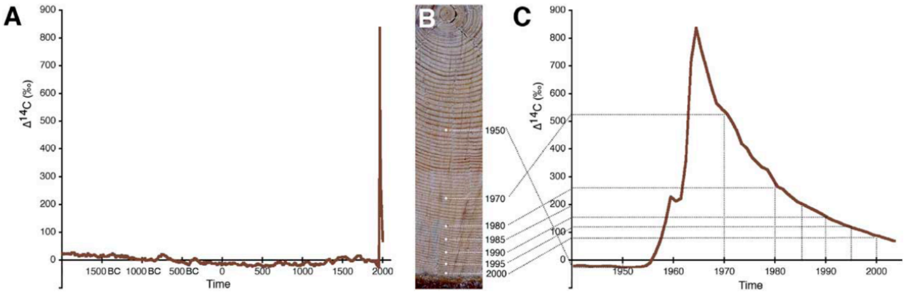


Figure 1.14: (A) Estimated ^{14}C composition of the atmosphere on a ~ 1000 yr time scale. (B) Cross section of a swedish pine tree, from which ^{14}C composition can be measured in successive rings, as shown in (C). Complied by KL Spalding, RD Bhardwaj, BA Buchholz, H Druid & J Frísen, *Cell* **122,** 133–145 (2005).

exponentially as it mixes with the oceans and biomass (Fig 1.14) Recently it has been suggested that this provides a signal that one can use, for example, to determine the birth dates of cells from different tissues in recently deceased people. While slightly macabre on several levels, this technique offers the opportunity to address really crucial questions such as whether we are growing new cells in our brain even when we are adults, or if all the cells in the brain are born more or less when we are born.

Problem 19: The radioactive isotope ^{14}C has a half–life of $t_{1/2} = 5730$ years. You find two human skeletons which you suspect are about $10,000$ years old. The setting in which you find these skeletons suggests that they died in two events separated by roughly 20 years. How accurately do you need to measure the abundance of ^{14}C in the skeletons in order to test this prediction? State as clearly as possible any assumptions that are made in interpreting such measurements.

If we want to look at events that take much longer than 5000 years, it's useful to look for radioactive decays that have much longer half lives. If you poke around the periodic table, you find that heavy elements often have radioactive isotopes with half lives measured in billions of years. Let's focus on the uranium isotopes which decay into lead. Specifically, ^{235}U decays into ^{207}Pb at a rate $\lambda_{235} = 9.849 \times 10^{-10}\,\text{yr}^{-1}$, while ^{238}U decays into ^{206}Pb at a rate $\lambda_{238} = 1.551 \times 10^{-10}\text{yr}^{-1}$:

$$^{235}\text{U} \overset{\lambda_{235}}{\rightarrow} {}^{207}\text{Pb} + \cdots \tag{1.130}$$

$$^{238}\text{U} \overset{\lambda_{238}}{\rightarrow} {}^{206}\text{Pb} + \cdots\,, \tag{1.131}$$

where in both reactions $\cdots$ refers to additional fragments that emerge in the fission of the uranium nucleus. If we imagine a hunk of rock that formed at time $t = 0$ in the distant past, then all of the uranium nuclei are decaying, so what we measure now at time t is

$$^{235}\text{U}(t) = {}^{235}\text{U}(0)\exp(-\lambda_{235}t) \tag{1.132}$$

$$^{238}\text{U}(t) = {}^{238}\text{U}(0)\exp(-\lambda_{238}t). \tag{1.133}$$

Every uranium nucleus that decays adds to the number of lead atoms that we find in the rock, so that

$$^{207}\text{Pb}(t) = {}^{207}\text{Pb}(0) + [{}^{235}\text{U}(0) - {}^{235}\text{U}(t)] \tag{1.134}$$

$$^{206}\text{Pb}(t) = {}^{206}\text{Pb}(0) + [{}^{238}\text{U}(0) - {}^{238}\text{U}(t)]. \tag{1.135}$$

Remember that we don't actually know what the isotopic compositions were when the rock was first formed. So in order to use these equations to analyze real data, we should try to get rid of all the terms that involve the isotopic compositions at $t = 0$.

We can start with uranium, for which everything we observe today is just a decayed version of where things started; this means that we can invert Eq's (1.132) and (1.133):

$$^{235}\text{U}(0) = {}^{235}\text{U}(t)\exp(+\lambda_{235}t) \tag{1.136}$$

$$^{238}\text{U}(0) = {}^{238}\text{U}(t)\exp(+\lambda_{238}t), \tag{1.137}$$

and then we can substitute into our equations for the current amount of the two lead isotopes [Eq's (1.134,1.135)] to obtain

$$^{207}\text{Pb}(t) = {}^{207}\text{Pb}(0) + [{}^{235}\text{U}(t)\exp(+\lambda_{235}t) - {}^{235}\text{U}(t)] \tag{1.138}$$

$$^{206}\text{Pb}(t) = {}^{206}\text{Pb}(0) + [{}^{238}\text{U}(t)\exp(+\lambda_{238}t) - {}^{238}\text{U}(t)], \tag{1.139}$$

or more simply

$$^{207}\text{Pb}(t) = {}^{207}\text{Pb}(0) + {}^{235}\text{U}(t)[\exp(+\lambda_{235}t) - 1] \tag{1.140}$$

$$^{206}\text{Pb}(t) = {}^{206}\text{Pb}(0) + {}^{238}\text{U}(t)[\exp(+\lambda_{238}t) - 1], \tag{1.141}$$

This is almost a relationship between things we can measure—the current numbers of atoms of each isotope—but not quite. First of all, we still have the initial concentrations of the lead isotopes. Second, it's hard to make absolute measurements (how could we be sure that we got all the lead out, as it were), so it would be nice to express things in terms of isotopic ratios.

The key idea is that different rocks start out with different amounts of lead and uranium, because that involves the chemistry of formation of the rock, but if all these heavy elements were made in a single event such as a supernova then the ratios of the isotopes would have been the same in all materials at $t = 0$. Since all that happens to the uranium nuclei is that they decay, the ratio of ^{235}U to ^{238}U still is the same in all materials, although of course it might be very different from the ratio at $t = 0$. To make use of this fact, let's try to solve for the number of ^{238}U atoms as a function of the number of ^{206}Pb atoms:

$$\begin{aligned} {}^{206}\mathrm{Pb}(t) &= {}^{206}\mathrm{Pb}(0) + {}^{238}\mathrm{U}(t)[\exp(+\lambda_{238}t) - 1] \\ \Rightarrow {}^{238}\mathrm{U}(t) &= \frac{{}^{206}\mathrm{Pb}(t) - {}^{206}\mathrm{Pb}(0)}{\exp(+\lambda_{238}t) - 1}. \end{aligned} \tag{1.142}$$

But if we measure the ratio $^{235}\mathrm{U}(t)/^{238}\mathrm{U}(t)$ today and call this ratio $R_{235/238}$, we can say that

$$^{235}\mathrm{U}(t) = R_{235/238}\frac{{}^{206}\mathrm{Pb}(t) - {}^{206}\mathrm{Pb}(0)}{\exp(+\lambda_{238}t) - 1}. \tag{1.143}$$

This relates the ^{235}U concentration in a sample to the ^{206}Pb concentration, both measured today. But we have seen that the ^{235}U concentration is related to the number of atoms of the *other* lead isotope, through Eq (1.140).

So we can put these equations together:

$$\begin{aligned}
{}^{207}\mathrm{Pb}(t) &= {}^{207}\mathrm{Pb}(0) + {}^{235}\mathrm{U}(t)[\exp(+\lambda_{235}t) - 1] \\
{}^{235}\mathrm{U}(t) &= R_{235/238}\frac{{}^{206}\mathrm{Pb}(t) - {}^{206}\mathrm{Pb}(0)}{\exp(+\lambda_{238}t) - 1} \\
\Rightarrow {}^{207}\mathrm{Pb}(t) &= {}^{207}\mathrm{Pb}(0) \\
&\quad + R_{235/238}\frac{{}^{206}\mathrm{Pb}(t) - {}^{206}\mathrm{Pb}(0)}{\exp(+\lambda_{238}t) - 1}[\exp(+\lambda_{235}t) - 1] \qquad (1.144) \\
&= {}^{207}\mathrm{Pb}(0) - {}^{206}\mathrm{Pb}(0)R_{235/238}\frac{\exp(+\lambda_{235}t) - 1}{\exp(+\lambda_{238}t) - 1} \\
&\quad + {}^{206}\mathrm{Pb}(t)\left[R_{235/238}\frac{\exp(+\lambda_{235}t) - 1}{\exp(+\lambda_{238}t) - 1}\right] \qquad (1.145)
\end{aligned}$$

This is an interesting equation, because it says that the amount of ${}^{207}\mathrm{Pb}$ that we find today in a rock should be related to the amount of ${}^{206}\mathrm{Pb}$ that we find in that same piece of rock. But we still have those pesky initial values to deal with.

There is yet a third isotope of lead which is both stable and *not* the product of other radioactive decays, and this is ${}^{204}\mathrm{Pb}$. So the amount of this isotope that we measure today is the same as we would have measured when the rock was formed. This means that we can take our expression for ${}^{207}\mathrm{Pb}(t)$ in Eq (1.145) and normalize by ${}^{204}\mathrm{Pb}(t)$,

$$\begin{aligned}
\frac{{}^{207}\mathrm{Pb}(t)}{{}^{204}\mathrm{Pb}(t)} &= \frac{{}^{207}\mathrm{Pb}(0)}{{}^{204}\mathrm{Pb}(t)} - \frac{{}^{206}\mathrm{Pb}(0)}{{}^{204}\mathrm{Pb}(t)}R_{235/238}\frac{\exp(+\lambda_{235}t) - 1}{\exp(+\lambda_{238}t) - 1} \\
&\quad + \frac{{}^{206}\mathrm{Pb}(t)}{{}^{204}\mathrm{Pb}(t)}\left[R_{235/238}\frac{\exp(+\lambda_{235}t) - 1}{\exp(+\lambda_{238}t) - 1}\right], \qquad (1.146)
\end{aligned}$$

but then we are free to rewrite ${}^{204}\mathrm{Pb}(t) \rightarrow {}^{204}\mathrm{Pb}(0)$ anyplace where it would make thing look better. So this last equation becomes

$$\begin{aligned}
\frac{{}^{207}\mathrm{Pb}(t)}{{}^{204}\mathrm{Pb}(t)} &= \frac{{}^{207}\mathrm{Pb}(0)}{{}^{204}\mathrm{Pb}(0)} - \frac{{}^{206}\mathrm{Pb}(0)}{{}^{204}\mathrm{Pb}(0)}R_{235/238}\frac{\exp(+\lambda_{235}t) - 1}{\exp(+\lambda_{238}t) - 1} \\
&\quad + \frac{{}^{206}\mathrm{Pb}(t)}{{}^{204}\mathrm{Pb}(t)}\left[R_{235/238}\frac{\exp(+\lambda_{235}t) - 1}{\exp(+\lambda_{238}t) - 1}\right], \qquad (1.147)
\end{aligned}$$

This looks complicated, but it's not. We can rewrite this equation as

$$\frac{{}^{207}\mathrm{Pb}(t)}{{}^{204}\mathrm{Pb}(t)} = A + B\frac{{}^{206}\mathrm{Pb}(t)}{{}^{204}\mathrm{Pb}(t)}, \qquad (1.148)$$

where the first important point is that A and B should be the same in all rocks (!).

Actually, Eq (1.148) contains a prediction of tremendous power. You should go back over the derivation and see what we had to assume:

- Uranium isotopes decay into lead isotopes as observed in the lab.
- Nothing else decays into lead, which is stable, and no processes produce any new uranium; again these are statements based on laboratory observations.
- All of the heavy elements that we find in our neighborhood were made at some moment $t = 0$ in the past, and this event set the initial isotopic ratios for each element.
- Different materials start with different amounts of uranium and lead.

Notice that the first two assumptions are based on direct measurements. The last item is the assumption that nothing special happens to force a relationship between the lead and uranium content of different materials, so it isn't really an assumption. The only really startling claim on the list is that all the heavy elements were made at some specific time in the past. So this assumption—literally a hypothesis about the creation of the materials in our local corner of the universe—makes a prediction about what we will see if we measure the isotopic composition of many different materials: if you plot $^{207}\mathrm{Pb}/^{204}\mathrm{Pb}$ vs $^{206}\mathrm{Pb}/^{204}\mathrm{Pb}$, you'll see a straight line. As you can see in Fig 1.15 this works!

One can in fact do a little more with the data from Fig 1.15 and related experiments. Our simple form in Eq (1.148) hides the fact that the constants A and especially B have meaning. Referring to Eq (1.147), we see that the slope B involves the current ratio $R_{235/238}$ of uranium isotopes, the decay rates λ_{235} and λ_{238} of the uranium isotopes, and the time t since the creation of the elements. All of these things except the time t have been measured independently. So, by analyzing the slop of the line in Fig 1.15, we determine the time that has elapsed since the heavy elements were formed. The result is $t = 4.55 \times 10^9\,\mathrm{yr}$. Even better is that you can do all this same analysis with other combinations of isotopes (e.g., rubidium and strontium) and you get the same answer for t even though everything else is different. This is impressive evidence that there really was some discrete event several billion years ago that created the heavy elements in our neighborhood.

Just to avoid confusion, what we have just calculated is *not* the time of the big bang. The heavy elements were formed only once the universe had

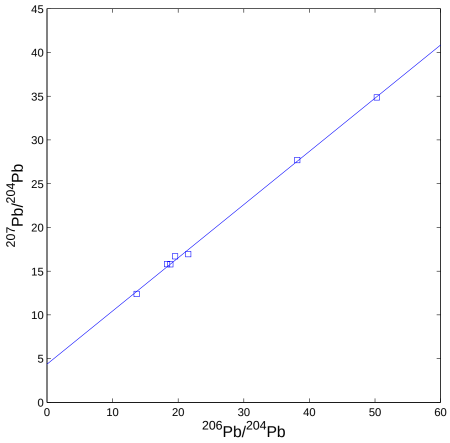


Figure 1.15: Isotopic compositions of some stone meteorites and terrestrial rocks. The fact that the data fall on a straight line is consistent with a single 'moment of creation' for the heavy elements, and the slope determines that this origin was 4.55×10^9 yr in the past. From data in V RamaMurthy & CC Patterson, Primary isochron of zero age for meteorites and the earth, *Journal of Geophysical Research* **67,** 1161 (1962).

developed to the point of having stars that could "cook" the light elements into more bigger nuclei. Actually, it's not automatic that these estimates for the age of heavy elements in the solar system should come out younger than the age of the universe as a whole (that is, the time since the big bang), which is estimated from very different kinds of data. There have been some tense moments in the history of the subject, but everything now is consistent; the big bang happened 13.7 billion years ago, with an uncertainty of about 1% (!).

It is worth remembering, at this point, that our whole line of argument leading to this remarkable conclusion hinges on the fact that we can solve the simple first order differential equation that describes radioactive decay. We know that this is the right equation because we have made measurements in the laboratory, but these measurements cover a range of (at best) a few years. Trusting the equations, we extrapolate the solutions over billions of years, and we obtain a wonderfully consistent view of the data.

An interesting question is whether there is any other evidence that the relevant parameters are constant over a period that is a significant fraction of the age of the universe. In fact, many people have considered the possibility that what we call "fundamental constants" of nature—including the constants that determine the rates of radioactive decay—might be changing slowly as the universe ages (and, as we now know, expands). Small rates of change obviously would have big consequences over such long time scales. For better or worse, there is no positive evidence for such changes, despite many ingenious, high precision measurements. This remains, however, a place where people are looking for cracks in our otherwise quite solid understanding.

Problem 20: The Allende chondrites are carbonaceous meteorites that fell near the town of that name in Mexico on February 8, 1969. Chondrites are a class of meteorites composed of tiny, rounded spheres containing silicate minerals (called chondrules). The chondrules are believed to have formed early in the solar nebula and many geochemical studies have been performed on them. Mass spectrometric data obtained from these chondrules has allowed the determination of their elemental compositions. Shown in Table 1.2 are typical data for isotope ratios of rubidium and strontium obtained by Gray and coworkers in 1973.

(a.) Derive a simple, integrated expression relating the age of such a sample to the isotope ratios.

(b.) Calculate the age of these samples from this data using the known half–life for radioactive decay of ^{87}Rb to ^{87}Sr of 48.8 billion years. Note that the strontium isotopes are stable and do not decay.

^{87}Rb/^{86}Sr	^{87}Sr/^{86}Sr
0.00014	0.698770
0.00019	0.698810
0.00075	0.698890
0.00393	0.698990
0.00432	0.699030
0.00660	0.699250
0.00776	0.699140
0.00853	0.699330
0.05213	0.702140
0.00017	0.698770

Table 1.2: Isotopic ratios from the Allende chondrites.

Intriguingly, these chondrites have been found to contain both natural and unnatural amino acids. But that is a topic for another day.

1.4 Using computers to solve differential equations

We have been looking so far at differential equations whose solutions can be constructed from "elementary functions," functions that we can write down in some simple form, look at and (hopefully) understand. In general, this isn't possible and in fact it might just be a historical artifact that certain functions have names and others don't. If you think you have the right equation to describe a system you are interested in, the fact that you can't immediately write down the solution shouldn't stop you. You can make approximations, which generates a lot of intuition, and you can use a computer to generate numerical solutions. This latter approach is general, and you should learn how to do it to the point where you feel comfortable.

Let us start with the simplest equation for first order chemical kinetics, in which some molecule A is tranformed into B with a rate constant k. The concentration c_A of A molecules obeys the equation

$$\frac{dc_A}{dt} = -kc_A. \tag{1.149}$$

As you all know by now, the solution is $c_A(t) = c_A(0)\exp(-kt)$. Let's see how we could find this solution numerically, check against the analytic solution to see that our strategy works, and finally use the same strategy to look at equations that are not so easy to solve with pen and paper.

Recall that the derivative is defined in calculus as the limit of finite differences:

$$\frac{dc_A(t)}{dt} \equiv \lim_{\Delta t \to 0} \frac{c_A(t+\Delta t) - c_A(t)}{\Delta t}. \tag{1.150}$$

The key to numerical solutions of differential equations is in essence to take a giant step backward and work with a finite value of Δt, hoping that we can make it small enough that we start to see the limiting behavior. In the simplest case we just make the replacement

$$\frac{dc_A}{dt} \rightarrow \frac{c_A(t+\Delta t) - c_A(t)}{\Delta t} \tag{1.151}$$

in the differential equation, and proceed:

$$\begin{aligned}
\frac{dc_A}{dt} \rightarrow \frac{c_A(t+\Delta t) - c_A(t)}{\Delta t} &= -kc_A(t) && (1.152)\\
c_A(t+\Delta t) - c_A(t) &= -[k\Delta t]c_A(t) && (1.153)\\
c_A(t+\Delta t) &= [1 - k\Delta t]c_A(t). && (1.154)
\end{aligned}$$

If we decide to measure time in discrete ticks of a clock, where the time between ticks is Δt, then every time $t = n \cdot \Delta t$, where $n = 0, 1, 2, 3, \ldots$. Thus instead of writing $c_A(t)$, we can write $c_A(n)$, and of course $c_A(t+\Delta t) = c_A(n+1)$. This means that Eq (1.154) really is an equation that generates $c_A(n+1)$ from knowledge of $c_A(n)$:

$$c_A(n+1) = [1 - k\Delta t]c_A(n). \tag{1.155}$$

If we start with some value of $c_A(0)$, Eq (1.155) tells us how to generate $c_A(1)$, and then we can use this iteratively to generate values for c_A at all discrete times n. In effect this allows us to "walk" through time, updating the value of c_A based on the previous value, and in this way we generate a "numerical solution" to our differential equations.

Let's see how this works in MATLAB. We'll choose units where the rate constant $k = 1$, and our "small steps of time" will be $\Delta t = 0.01$; we'll have to come back to the question of whether this choice of Δt is a good one. We'll explore times starting at $t = 0$ and ending at $t = 5$ (again, in units where $k = 1$), which means that we need to run for 500 ticks of our discrete clock. With these remarks in mind, the program becomes

```
cA = zeros(500,1);
cA(1) = 1;
k = 1;
dt = 0.01
for n=2:length(cA);
     cA(n) = (1-k*dt)*cA(n-1);
end;
```

Notice that we start by setting aside space for the thing we trying to compute, and we have to set (in the second line) its initial value. A peculiarity of MATLAB is that you start counting at `n=1`, not at `n=0`. We also have lines which define the value of the rate constant `k` and time step Δt, which is symbolized by `dt` in the program; again, our choices of these parameters are just for illustration at the moment. Once you run the program you have stored the "data" on concentration as a function of time, and you'd like to plot it. If you want things in physical units it's convenient to make a real time axis,

```
timeaxis = dt*[0:499];
```

where we are careful to note that the time corresponding to `n=1` is actually $t = 0$. Then you can type

```
figure(1)
plot(timeaxis,cA)
xlabel('time (seconds)')
ylabel('concentration of A')
```

and you should get a reasonable plot with properly labeled axes, and this will appear on your screen in a box marked Figure 1. This is not the place for aesthetic hints, but at some point you'll want to learn how to make things look nice—what is important here is to be sure that when you look at the plot you can read the units! The results are shown in Fig 1.16, where we compare the numerical solution to a numerical evaluation of the analytical result. In this simple case, it's clear that our numerical strategy "works," in that it gives us a solution that agrees with the exact mathematics.

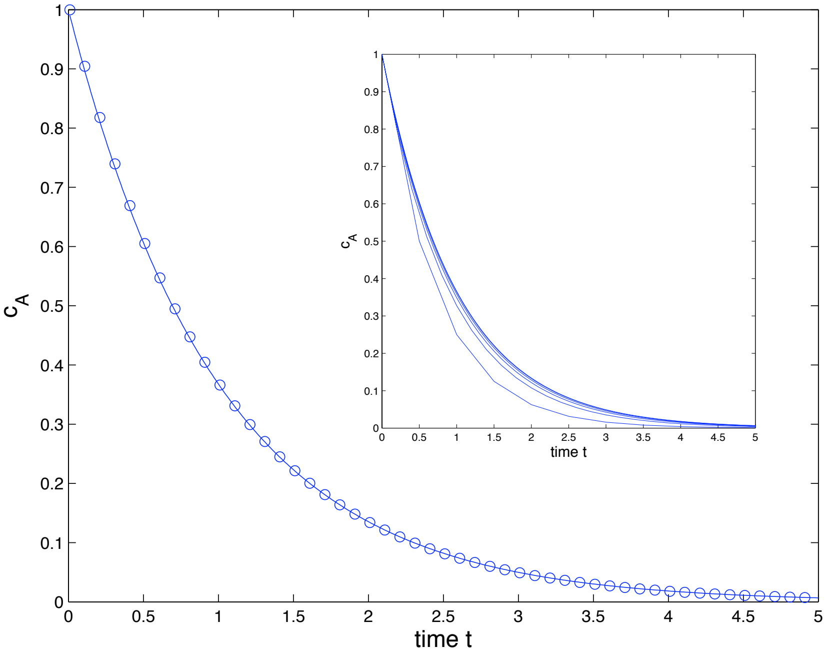


Figure 1.16: Numerical solution of the simple differential equation, Eq (1.149). As described in the text we use the algorithm defined by Eq (1.155), with the rate constant $k = 1\,\mathrm{s}^{-1}$ and the initial condition $c_A(1) = 1$ (in some units). The solid line is the result of 500 iterations with $\Delta t = 0.01\,\mathrm{s}$, and the circles show the exact solution over the same time window. Inset shows what happens as we increase Δt, with separate curves for $\Delta t = 0.01$, 0.02, 0.05, 0.1, 0.2, 0.5.

We have of course chosen here a VERY simple example. In particular we have an exact analytical solution, so using the computer is just for the sake of learning how to do it. In the problems we ask you to play a bit, changing parameters to see what is essential in making things work. In the approach suggested here, the basic issue is how to choose the size of the discrete time step `dt`. The whole idea behind our scheme is to replace derivatives with differences, and this gets to be a bad approximation if we make our steps too big, as you can see in the inset of Fig 1.16. So this pushes us toward smaller and smaller values of `dt`. But if we take very small steps then we need to take lots of steps to cover the same amount of real time, and so our computation becomes inefficient.

Thanks to the increasing speed of the devices in your computer's chips, running programs for many time steps is less of a problem than it used to be, but still there are many situations in which one will need to push the tradeoff between accuracy and efficiency. To do this, one needs to understand something about the problem you are solving, but one can also try to use more intelligent mappings from the continuous differential equation down to the discrete time steps. This is a whole field of research (numerical analysis), and as time permits we'll give you glimpses. For now, it would be good if you felt comfortable with the simplest approaches, so that faced with some new differential equation you don't how to solve, you can go to the computer and quickly see what the solutions look like—and have ways of testing to see if you believe what the computer is telling you!

Problem 21: The basic idea of this section has been to take the differential equation

$$\frac{dc(t)}{dt} = -kc(t), \tag{1.156}$$

replace it with a discrete equation

$$\begin{aligned} \frac{c(t+\Delta t) - c(t)}{\Delta t} &= -kc(t) & (1.157)\\ \Rightarrow c(t+\Delta t) &= (1 - k\Delta t)c(t), & (1.158) \end{aligned}$$

and then turn this rule directly into an algorithm.

(a.) Consider the case where $k = 10\,\mathrm{s}^{-1}$. Try various values for Δt (e.g., $\Delta t = 0.001,\ 0.01,\ 0.1,\ 1\,\mathrm{s}$) and run your program for a number of iterations that corresponds to one second of real time. Compare your numerical results with the analytic solution $c_A(t) = c_A(0)\exp(-kt)$. How small does Δt need to be in order to get the right answer? How would your answer change if the rate k were ten times faster?

(b.) Write the analogous program for a second order reaction, $A + B \overset{k_2}{\rightarrow} C$, described by the differential equations

$$\frac{dc_A}{dt} = -k_2 c_A c_B \tag{1.159}$$

$$\frac{dc_B}{dt} = -k_2 c_A c_B. \tag{1.160}$$

(c.) Assume initial concentrations of $c_A(0) = 1\,\text{mM}$ and $c_B(0) = 2\,\text{mM}$. Let $k_2 = 10^6\,\text{M}^{-1}\text{s}^{-1}$. Before you run your program, what value of Δt seems reasonable? For how long (in real time) will you need to run in order to see most of the interesting dynamics?

(d.) Run your program using the parameter settings from part [c]. Is there an analytic solution to which you can compare your results? If you don't have such a solution, how do you decide whether your program is giving the right answer?

Problem 22: Let's try to use these ideas to solve the equations for motion under the influence of gravity. Going back to the discussion in Section 1.1, if the height of a particle with mass m is given by $h(t)$, then Netwon's equation becomes

$$m\frac{d^2h}{dt^2} = -mg, \tag{1.161}$$

again in the limit where we take the force of gravity to be constant. Since we have discussed ways of solving equations with one derivative, but not two derivatives, let's rewrite this as two equations:

$$\frac{dh}{dt} = v, \tag{1.162}$$

$$\frac{dv}{dt} = -g. \tag{1.163}$$

Notice that units are arbitrary. Suppose that we define variables $\tilde{h} = h/h_0$, $\tilde{t} = t/t_0$, and $\tilde{v} = v/v_0$, where we choose the velocity scale to be the initial velocity, $v_0 = v(0)$.

(a.) Write the differential equations for these new variables, that is

$$\frac{d\tilde{h}}{d\tilde{t}} = \cdots, \tag{1.164}$$

$$\frac{d\tilde{v}}{d\tilde{t}} = \cdots. \tag{1.165}$$

(b.) Show that by choosing the scales h_0 and t_0 correctly, you can make even the constant g disappear from the equations. What does this mean, qualitatively, about the form of the solutions to these equations?

(c.) Write a program to solve these "dimensionless" equations, discretizing into time steps of size Δt as before. Run the program, and compare your results with the exact solution from the discussion in Section 1.1.

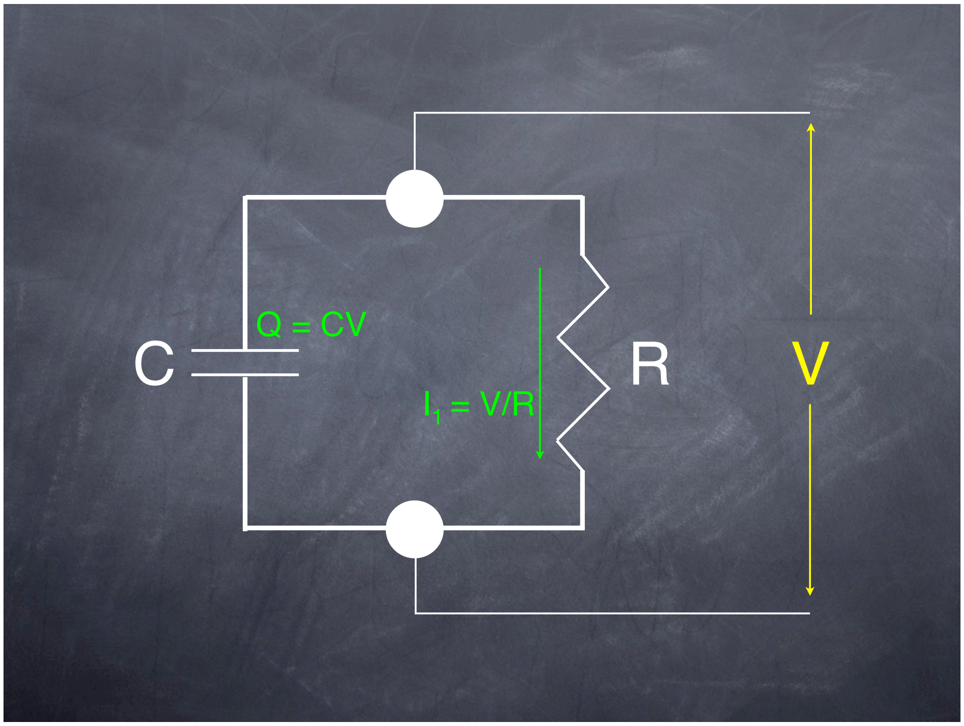


Figure 1.17: A capacitor C and resistor R connected in parallel. The voltage drop V is the same across the two elements of the circuit, while the currents flowing through the two circuit element must add to zero, as expressed in Eq (1.166).

1.5 Simple circuits and population dynamics

Most of you remember a little bit about electrical circuits from your high school physics classes. In Fig 1.17 we show a capacitor C and a resistor R connected in parallel. Here "parallel" means that the voltage difference V between the two plates of the capacitor is the same as the voltage difference across the resistor. In this simple case the circuit is closed and there is no path for current to flow out, so the current that flows through the capacitor and resistor must add up to zero. This condition of zero current (an application of Kirchoff's laws, if that jogs your memory) allows us to write down the equation for the dynamics of the voltage V in this circuit.

Recall that the current which flows through the resistor is just $I_1 = V/R$. We usually think of the capacitor as being described by $Q = CV$, where Q is the charge on the capacitor plates, but of course if the charge changes with time there is a current flow (by definition), so that the current which flows through the capacitor is $I_2 = d(CV)/dt = C(dV/dt)$. Adding these currents must give zero, and this must be true at every moment of time t:

$$I_1 + I_2 = \frac{V(t)}{R} + C\frac{dV(t)}{dt} = 0. \tag{1.166}$$

It is slightly more convenient to write this as

$$RC\frac{dV(t)}{dt} + V(t) = 0. \tag{1.167}$$

We recognize Eq (1.167) as the same equation we have seen before, both in the mechanics of motion with drag and in first order chemical kinetics. By now we know that the solution is an exponential decay,

$$V(t) = V(0)e^{-t/\tau}, \tag{1.168}$$

where the time constant $\tau = RC$. As you might guess by looking at the circuit—there is no battery and no current source—any initial voltage $V(0)$ decays to zero, and this decay happens on a time scale $\tau = RC$. This is important because most circuits that we build, including the circuits on the chips in your computer, have some combination of resistance and capacitance, and so we know that there is a time scale over which these circuits will lose their memory. In memory chips we want this to be a very long time, so (roughly speaking) one tries to design the circuit so that R is very large. Conversely, on the processor chips things should happen fast, so RC should be small. You may recall that the capacitance C is determined largely by geometry—how big are the plates and how far apart are they?—so if we want to squeeze a certain number of circuit elements into a given area of the chip the capacitances are more or less fixed, and the challenge is to reduce R.

Almost the same equations arise in a very different context, namely population growth. Imagine that we put a small number of bacteria into a large container, with plenty of food; you will soon do more or less this experiment in the lab part of the course. Let's call $n(t)$ the number of bacteria present at time t. Because the bacteria divide, $n(t)$ increases. As a first approximation, it's plausible that the rate at which new bacteria appear is proportional to the number of bacteria already there, so we can write

$$\frac{dn(t)}{dt} = rn(t), \tag{1.169}$$

where r is the "growth rate." This is just like the equations we have seen so far, but the sign is different.

When we had an equation of the form

$$\frac{dx}{dt} = -kx, \tag{1.170}$$

we found that the solution is of the form $x(t) = A\exp(-kt)$, where the constant $A = x(t = 0)$. More generally we can say that this solution is of the form $x(t) = A\exp(\lambda t)$, and it turns out the $\lambda = -k$. As will become clearer in the next few lectures, this exponential form is very general, and helps us solve a large class of problems. So, let's try it here.

We guess a solution in the form $n(t) = Ae^{\lambda t}$, and substitute into Eq (1.169):

$$\begin{aligned} \frac{dn(t)}{dt} &= rn(t) \\ \frac{d}{dt}[Ae^{\lambda t}] &= r[Ae^{\lambda t}] && (1.171) \\ A\frac{d}{dt}[e^{\lambda t}] &= && (1.172) \\ A\lambda[e^{\lambda t}] &= Ar[e^{\lambda t}]. && (1.173) \end{aligned}$$

Now the exponential of any finite quantity can never be zero, so we can divide both sides of the equation by $[e^{\lambda t}]$ to obtian

$$\begin{aligned} A\lambda[e^{\lambda t}] &= Ar[e^{\lambda t}] \\ A\lambda &= Ar. && (1.174) \end{aligned}$$

As for the constant A, if this is zero we are in trouble, since then our whole solution is zero for all time (this is sometimes called the "trivial" solution; we'll try to avoid using that word in this course). So we can divide through by A as well, and we find that $\lambda = r$. The important point is that by choosing an exponential form for our solution we turned the differential equation into an algebraic equation, and in this case even the algebra is easy. So we have shown that the population behaves as $n(t) = Ae^{\lambda t}$, where $\lambda = r$ and you should be able to show that A is the population at $t = 0$, so that

$$n(t) = n(0)e^{rt}. \tag{1.175}$$

Thus, rather than decaying exponentially, the population of bacteria grows exponentially with time. Instead of a half–life we now have a doubling time $\tau_{\text{double}} = \ln 2/r$, which is the time required for the population to become twice as large.

We have (perhaps optimistically) ignored death. But death only happens to bacteria that are alive (!), so again its plausible that the rate at which the population *decreases* by death is proportional to the number of bacteria, $-dn(t)$, where d is the death rate. Then

$$\frac{dn(t)}{dt} = rn(t) - dn(t) = (r - d)n(t), \tag{1.176}$$

so if we define a new growth rate $r' = r - d$ everything is as it was before. In fact, if we are just watching the total number of bacteria we can't tell the difference between a slower growth rate and a faster death rate.

These equations for the population of bacteria are approximate. Let's make a list of some of the things that we have ignored, and see if we can improve our approximation:

- We've assumed that the discreteness of bacteria isn't important—you can't have 305.7 bacteria, but we pretend that $n(t)$ is a continuous function. Probably this isn't too bad if the population is of a reasonable size.
- We've assumed that all the bacteria are the same. It's not so hard to make sure that they are genetically identical—just start with one and don't let things run long enough to accumulate too many mutations. It takes more effort to insure that all the bacteria experience the same environment.
- We've assumed that the bacteria don't murder each other, and more gently that the consumption of food by the ever increasing number of bacteria doesn't limit the growth.
- We've assumed that the growth isn't synchronized.

These last two points deserve some discussion.

We can model the "environmental impact" of the bacteria by saying that the effective growth rate r' gets smaller as the number of bacteria gets larger. Certainly this starts out being linear, so maybe we can write $r' = r_0[1 - an(t)]$, so that

$$\frac{dn(t)}{dt} = r_0[1 - an(t)]n(t). \tag{1.177}$$

But then this defines a critical population size $n_c = 1/a$ such that once $n = n_c$ the growth will stop ($dn/dt = 0$)—the environment has reached its capacity for sustaining the population. It's natural to measure the population size as a fraction of this capacity, so we write $x = n/n_c$, so (being careful with all the steps, since this is the kind of thing you'll need to do many times)

$$\begin{aligned}
\frac{dn(t)}{dt} &= r_0[1 - an(t)]n(t) \\
\frac{d}{dt}\left(n_c\frac{n(t)}{n_c}\right) &= r_0\left[1 - a\left(n_c\frac{n(t)}{n_c}\right)\right]\left(n_c\frac{n(t)}{n_c}\right) \qquad (1.178) \\
n_c\frac{dx(t)}{dt} &= r_0[1 - (an_c)x(t)]n_c x(t) \qquad (1.179) \\
\frac{dx(t)}{dt} &= r_0 x(t)[1 - x(t)], \qquad (1.180)
\end{aligned}$$

where at the last step we cancel the common factor of n_c and use the fact that (by our choice of n_c) $an_c = 1$.

This equation predicts that if we start with a very small ($x \ll 1$) population, the growth will be exponential with a rate r_0, but as x gets close to 1 this has to stop, and the population will reach a steady, saturated state. These dynamics will be important in your experiments, so let's actually solve this equation.

Problem 23: In the previous paragraph we made some claims about the behavior of $x(t)$, based on Eq (1.180), but without actually solving the equation (yet). Can you explain why these claims are true, also without constructing a full solution? To get started, can you make a simpler, approximate equation that should describe the dynamics accurately when $x \ll 1$?

We use the same idea as before, "moving" the x's to one side of the equation and the dt to the other:

$$\begin{aligned}
\frac{dx}{dt} &= r_0 x[1 - x] \qquad (1.181) \\
\frac{dx}{x(1-x)} &= r_0 dt. \qquad (1.182)
\end{aligned}$$

If you remember how to do the integral

$$\int \frac{dx}{x(1-x)},$$

you can proceed directly from here. If, like me, you remember that

$$\int \frac{dx}{x} = \ln x,$$

but aren't sure what to do about the more complicated case, then you need to turn the problem you have into the one you remember how to solve.

Problem 24: Starting with

$$\int \frac{dx}{x} = \ln x, \tag{1.183}$$

remind yourself of why

$$\int \frac{dx}{1-x} = -\ln(1-x). \tag{1.184}$$

The trick we need here is that fractions which have products in the denominator can be expanded so that they just have single terms in the denominator. What this means is that we want to try writing

$$\frac{1}{x(1-x)} = \frac{A}{x} + \frac{B}{1-x}, \tag{1.185}$$

but we have to choose A and B correctly. The way to do this is to work backwards:

$$\begin{aligned} \frac{A}{x} + \frac{B}{1-x} &= \frac{A(1-x)}{x(1-x)} + \frac{Bx}{x(1-x)} && (1.186) \\ &= \frac{A(1-x)+Bx}{x(1-x)} && (1.187) \\ &= \frac{A+(B-A)x}{x(1-x)}. && (1.188) \end{aligned}$$

Now it is clear that if we want this to equal

$$\frac{1}{x(1-x)},$$

then we have to choose $A = 1$ and $B = A = 1$. So we have

$$\frac{1}{x(1-x)} = \frac{1}{x} + \frac{1}{1-x}, \tag{1.189}$$

and now we can go back to solving our original problem:

$$\begin{aligned}
\frac{dx}{x(1-x)} &= r_0 dt \\
\frac{dx}{x} + \frac{dx}{1-x} &= r_0 dt \qquad (1.190) \\
\int_{x(0)}^{x(t)} \frac{dx}{x} + \int_{x(0)}^{x(t)} \frac{dx}{1-x} &= \int_0^t r_0 dt \qquad (1.191) \\
\ln(x)\bigg|_{x(0)}^{x(t)} - \ln(1-x)\bigg|_{x(0)}^{x(t)} &= r_0 t \qquad (1.192) \\
\ln[x(t)] - \ln[x(0)] - \ln[1-x(t)] + \ln[1-x(0)] &= r_0 t \qquad (1.193) \\
\ln\left[\frac{x(t)}{x(0)} \cdot \frac{1-x(0)}{1-x(t)}\right] &= r_0 t \qquad (1.194) \\
\frac{x(t)}{x(0)} \cdot \frac{1-x(0)}{1-x(t)} &= \exp(r_0 t) \qquad (1.195) \\
\frac{x(t)}{1-x(t)} &= \frac{x(0)}{1-x(0)} \exp(r_0 t). \qquad (1.196)
\end{aligned}$$

Note that in the last steps we use the fact that sums (differences) of logs are the logs of products (ratios), and then we get rid of the logs by exponentiating both sides of the equation. The very last step puts the time dependent $x(t)$ on left side and the initial condition on the right.

Equation (1.196) is almost what we want, but it would be more useful to write $x(t)$ explicitly. Notice that what we have is of the form

$$\frac{x(t)}{1-x(t)} = F, \tag{1.197}$$

where F is some factor. You'll see things like this again, so it might be worth knowing the trick, which is to invert both sides, rearrange, and invert again:

$$\begin{aligned}
\frac{x(t)}{1-x(t)} &= F \\
\frac{1-x(t)}{x(t)} &= \frac{1}{F} && (1.198) \\
\frac{1}{x(t)} - 1 &= && (1.199) \\
\frac{1}{x(t)} &= 1 + \frac{1}{F} && (1.200) \\
&= \frac{F+1}{F} && (1.201) \\
x(t) &= \frac{F}{1+F}. && (1.202)
\end{aligned}$$

Armed with this little bit of algebra, we can solve for $x(t)$ in Eq (1.196):

$$\begin{aligned}
\frac{x(t)}{1-x(t)} &= \frac{x(0)}{1-x(0)} \exp(r_0 t) \\
\Rightarrow x(t) &= \frac{\frac{x(0)}{1-x(0)} \exp(r_0 t)}{1 + \frac{x(0)}{1-x(0)} \exp(r_0 t)} && (1.203) \\
&= \frac{x(0) \exp(r_0 t)}{[1-x(0)] + x(0) \exp(r_0 t)}, && (1.204)
\end{aligned}$$

where the last step is just to make things look a little nicer.

Some graphs of Eq (1.204) are shown in Fig 1.18. You should notice that all of the curves run smoothly from $x(0)$ up to the maximum value of $x = 1$ at long times. Indeed, all the curves seem to look the same, just shifted along the time axis. Hopefully you'll something like this in the lab!

Problem 25: It's useful to look at a expression like Eq (1.204) and "see" some of the key features that appear in the graphs, without actually making the exact plots.

(a.) Be sure that if you evaluate $x(t)$ at $t = 0$ you really do get $x(0)$, as you should if we did all the manipulations correctly.

(b.) Ask yourself what happens as $t \to \infty$. You should be able to see that $x(t)$ approaches 1, no matter what the initial value $x(0)$, as long as it's not zero.

(c.) Show that you rewrite Eq (1.204) as

$$x(t) = \frac{1}{1 + \exp[-r_0(t - t_0)]}, \qquad (1.205)$$

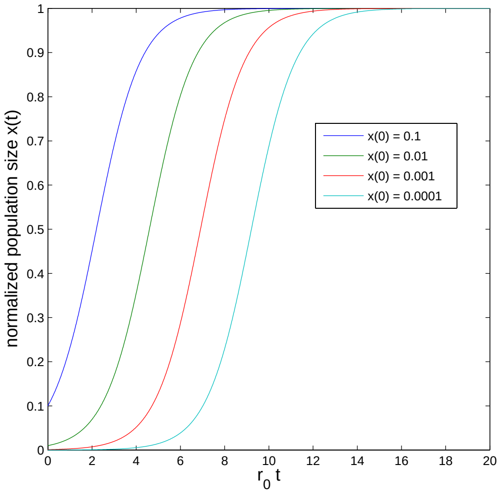


Figure 1.18: Dynamics of population growth as predicted by Eq (1.204), the solution to Eq (1.180). Time is measured in units of the growth rate r_0 of small populations, and the population size is normalized the "capacity" of the environment.

where t_0 depends on the initial population. What does this mean about the growth curves that start with different values of $x(0)$?

Problem 26: As discussed in connection with the first laboratory and in Section 1.1, an object moving through a fluid at relatively high velocities experiences a drag force proportional to the square of its velocity. In the presence gravity this means that $F = ma$ can be written as

$$m\frac{dv}{dt} = -av^2 + mg, \tag{1.206}$$

where the velocity v is positive if the object is moving downwards, a is the drag coefficient, and g as usual is the acceleration due to gravity. As noted in the lectures, a similar equations can arise in chemical kinetics.

(a.) For any given system, the usual units of time, speed, etc. might not be very natural. Perhaps there is some natural time scale t_0 and a natural velocity scale v_0 such that if we measure things in these units our equation will look simpler. Specifically, consider variables $u \equiv v/v_0$ and $\tau \equiv t/t_0$. Show that by proper choice of t_0 and v_0 one can make all the parameters (m, g, a) disappear from the differential equation for $u(\tau)$.

(b.) Solve the differential equation for $u(\tau)$. Does this function have a universal shape? Since we have gotten rid of all the parameters, is there anything left on which the shape could depend? If you need help doing an integral it's OK to use a table (or perhaps an electronic equivalent), but you need to give references. Translate your results into predictions about $v(t)$.

(c.) Suppose that the initial velocity $v(t = 0)$ is very close to the terminal velocity $v_\infty = \sqrt{mg/a}$. Show that your exact solution for $v(t)$ is approximately an exponential decay back to the terminal velocity. Then go back to Eq (1.206) and write $v(t) = v_\infty + \delta v(t)$, and make the approximation that δv is small, and hence δv^2 is even smaller and can be neglected. Can you now show that this approximate equation leads to an exponential decay of $\delta v(t)$, in agreement with your exact solution?

(d.) Explain the similarities between this problem and the population growth problem that starts with Eq (1.180) and leads to the results in Fig 1.18. Can you make an exact mapping from one problem to the other?

What about synchronization? Cell growth and division is a cycle, and if this cycle runs like a clock then we can imagine getting all the clocks aligned so that the population of bacteria holds fixed for some length of time, then doubles as all the cells proceed complete their cycle, then holds fixed, doubles again, and so on. In fact, real single celled organisms lose their synchronization if they don't communicate. On the other hand, many organisms (including big complicated ones not so different from us) get synchronized by the seasons—we are all familiar with the nearly simultaneous appearance of all the baby birds at the same time of year. This suggests that rather than writing down a differential equation, we should use one year as the natural unit of time and ask how the number of organisms in one year $n(t)$ depends on the number that were there last year $n(t-1)$. Again if we just think about growth we would argue that the number of new organisms if proportional to the number that we started with, hence

$$n(t) = Gn(t-1), \tag{1.207}$$

where $G > 1$ means that we are describing growth from season to season while $G < 1$ means that the population is dying out. It's interesting that in this case the seasonal synchronization doesn't make any difference, because the solution still is exponential: $n(t) = n(0)e^{t/\tau}$, where $\tau = 1/(\ln G)$.

Problem 27: Verify that Eq (1.207) is solved by $n(t) = n(0)e^{t/\tau}$, with $\tau = 1/(\ln G)$. As a prelude to things which will be important in the next major section of the course, consider a population in which some fraction of the organisms wait for two seasons to reproduce, so that

$$n(t) = G_1 n(t-1) + G_2 n(t-2). \tag{1.208}$$

Can you still find a solution of the form $n(t) \propto e^{t/\tau}$? If so, what is the equation that determines the value of the time constant τ?

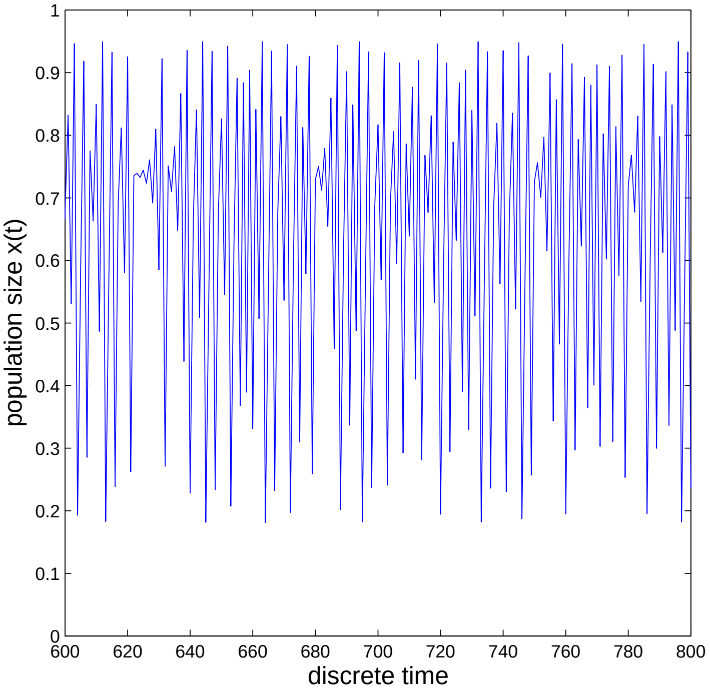


Figure 1.19: Simulation of Eq (1.209) with $G_0 = 3.8$ starting from an initial conditon $x(1) = 0.1$. This is in the chaotic regime. We see a general alternation from odd to even times, but no true periodicity.

Really interesting things happen when we combine the discreteness of seasons with the impact of other organisms on the growth rate. As before, we can try a linear approximation, so that $G = G_0[1 - n(t)/n_c]$, and we can rewrite everything in terms of the fractional population x:

$$x(t) = G_0 x(t-1)[1 - x(t-1)]. \tag{1.209}$$

If $G_0 < 1$, no matter where we start, eventually the population dies out and we approach $x = 0$ at long times. If G_0 is somewhat bigger than 1, then a small initial population grows and eventually saturates. But if G_0 gets even bigger, some interesting things happen. For example, when $G_0 = 3$, the population oscillates from season to season, being alternately large and small, and this oscillation continues forever—there is no decay or growth to a steady state. When $G_0 = 3.5$, there is an oscillation with alternating seasons of large and small population, but it takes a total of four seasons before the population repeats exactly. We say that at $G_0 = 3$ we observe a "period 2" oscillation, and at $G_0 = 3.5$ we observe a "period 4" oscillation. If we keep increasing G_0 we can observe period 8, period 16, ... all the powers of 2 (!). The transitions to longer and longer periods come more quickly as G_0 increases, until we exceed a critical value of G_0 and the trajectories $x(t)$ start to look completely random, even though they are generated by the simple Eq (1.209); see Fig 1.19.

Problem 28: Write a program to generate the trajectories $x(t)$ that are predicted by Eq (1.209). Run this program, exploring different values of G_0, and verify the statements made in the previous paragraph. In particular, try starting with different initial conditions $x(0)$, and see whether the solutions are "attracted" to some simple for at long times, or whether trajectories that start with slightly different values of $x(0)$ end up looking very different from each other. Does this dependence on initial conditions vary with the value of G_0? Can you see what this might have to do with the problem of predicting the weather?

The random looking trajectories of Fig 1.19 are called *chaotic*, and the discovery that such simple deterministic equations can generate chaos changed completely how we look at the dynamics of the world around us. What is remarkable is that the surprising properties of this simple equation (which you can rediscover for yourself even with a pocket calculator) are provably the properties of a broad class of equations, and one can observe the sequence of period doublings and the resulting chaos in real physical systems, matching quantitatively the predictions of the simple model to key features of the data.

This has been a scant introduction to a rich and beautiful subject. Please ask for more references if you are intrigued.

1.6 The complexity of DNA sequences

The native form of DNA is the famous double helix proposed by Watson and Crick in 1953. Most of the essential properties of DNA are inherent in its chemical structure. DNA is a polymer, that is a molecule constructed as a chain of (almost) repeating subunits. In particular, DNA is a high polymer, with huge numbers of the these subunits—in the human genome, there are individual DNA molecules that are 50 to 250 million units long, so that if we could stretch out these single molecules they would have lengths on the order of a meter or more. A strand is comprised of a covalent sugar-phosphate backbone, on which reside four chemically different structure called "bases," namely adenine (A), guanine (G), cytosine (C) and thymine (T). The two strands are held together by non–covalent hydrogen bonds between pairs of bases: A only pairs with T and G only pairs with C. The two strands are opposite in chemical orientation; by convention, sequences are read from the so–called 5' end.[6] If we think of one strand as having the base sequence 5' AGGCTC 3' then the other, complementary strand in native DNA will have the sequence 5' GAGCCT 3'.

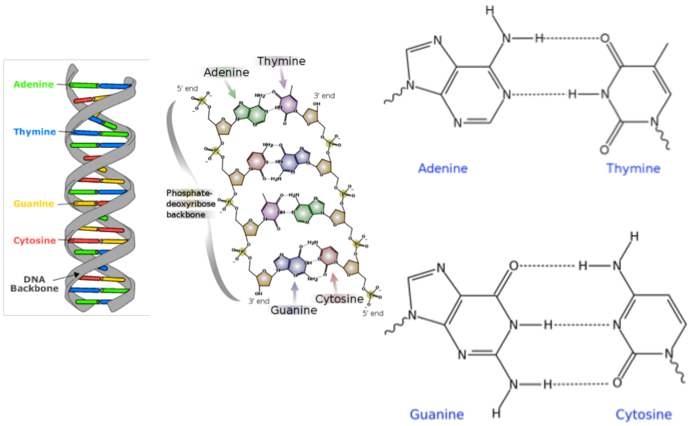


Figure 1.20: Three views of base pairing in the double helix.

Let us consider the relative strengths of the bonds in DNA. The strongest are the covalent bonds, such as the carbon–carbon, carbon–oxygen, and oxygen–phosphorus bonds that make up the backbone of each strand and between the backbone and the bases. Weaker bonds, called hydrogen bonds, connect the two strands. One can see, in the diagram of the base pairs, that hydrogen bonds consist of a hydrogen atom that is shared between a partially

---

[6] 3' and 5' refer to the conventional numbering scheme for the carbon atoms in the sugar residues along the backbone.

negatively-charged atom on a base in one strand and a partially positively-charged atom on the other. It should also be clear that the base-pairing rules are the consequence of the chemical features that allow the formation of stable hydrogen bonds only between A and T or C and G. It is also worth noting that A and G (called "purines") are bigger than C and T (called "pyrimidines"). Each of the basepairs has one large base (purine) and one small one (pyrimidine) such that when one basepair is stacked on another in the double-helical structure, the distance across them is the same, providing a constant inter-chain backbone distance. Making paper cutouts of the base pairs and trying to superimpose them (as Jim Watson describes he did in 1952) makes the structural constraints clear even to non–chemists.

In general, when we raise the temperature, molecules can access states with higher energy. In particular, since forming a bond lowers the energy, we expect that bonds will break as we heat things up. The weakest bonds break first, so at reasonable temperatures hydrogen bonds will be broken, while it would take much higher temperatures to break covalent bonds. Thus, as we heat up a DNA molecule, the hydrogen bonds that connect the two strands of the double helix break, but the strands themselves remain intact—the two strands of the double helix begin to separate, the double stranded DNA molecule becomes two single stranded molecules, and the DNA is said to be "denatured." Crucially, the two single stranded molecules that emerge from a double helix after denaturation have a special relationship: their nucleotide sequences are different, but complementary. Each single strand contains the same genetic information, which becomes clear when one thinks about what happens when each of the strands is copied using the base-pairing rules: copying either of the complementary strands will produce exactly the same double helix.

In the double–helical structure of DNA, each successive base pair is stacked on the previous one. The stacking is energetically favorable, and this contributes to the stability of the DNA structure. The stacking has another consequence: the optical properties of the DNA in the ultraviolet region of the spectrum are changed. When the bases are freer to tumble and turn in solution, they absorb more UV light than when there are stacked and conformationally constrained. This works, more or less, base by base, so if we monitor the absorption of light at a wavelength of $\lambda = 260\,\text{nm}$ we are essentially counting the fraction of bases that are stacked. If the only available states are single stranded (denatured) and double stranded, then this absorption A_{260} measures the fraction of denatured molecules, as in Fig 1.21; this is a very convenient way to follow DNA denaturation experimentally. As DNA denatures, the UV absorbance (A_{260}) rises, until it reaches a

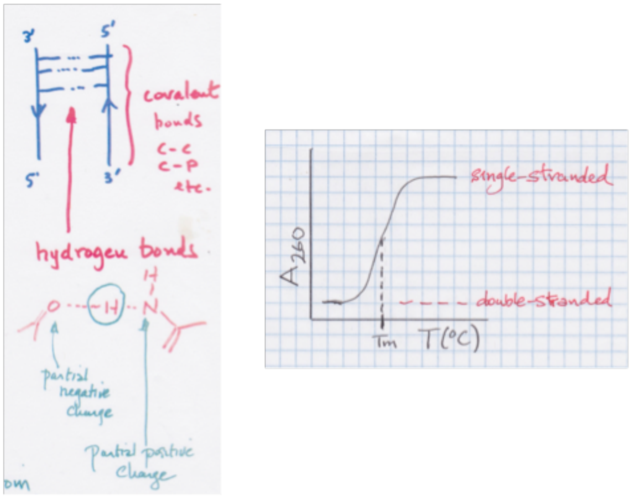


Figure 1.21: At left, a schematic of the hydrogen bonds the hold the two strands of DNA together. At right, the ultraviolet absorption (at a wavelength $\lambda = 260\,\text{nm}$) of a DNA sample as a function of temperature. As the molecule melts, we see a transition from weak absorption by double stranded DNA to stronger absorption by single stranded DNA.

maximum when all the strands have been separated and no double-stranded molecules are left. The melting temperature (T_{m}) is defined as the temperature at which, under standard conditions half of the DNA is denatured and half is still in the native double stranded conformation.

Because the two strands the emerge from denaturing double stranded DNA contain complementary sequences of bases, these individual strands carry the information needed to find one another again, and remake the correct hydrogen bonds, if we lower the temperature. This process, undoing the denaturation, is called renaturation, annealing, or reassociation; if we don't have precisely complementary strands, many of the bonds still can form, and this is called hybridization. Importantly, the renaturation reaction requires nothing except the two strands, and appropriate conditions of salt, pH and temperature. The standard conditions for renaturation are temperature lower than, but near T_{m}, relatively high salt and nearly neutral pH. Under these conditions renaturation requires that the sequences of the two strands be very close to exact complementarity. Conditions can readily be found such that even a single mismatched basepair can effectively prevent renaturation in molecules of considerable length.

It is this intrinsic ability of DNA molecules to distinguish differences in nucleotide sequences during renaturation or hybridization that is the basis for accurate information transfer during the basic genetic processes required of all cells: i.e. replication of the DNA, transcription of expressed gene sequences into RNA, and translation of mRNA into proteins. Furthermore, virtually every technique and method in modern molecular biology depends ultimately on this property of DNA and RNA.

Figure 1.21 shows us how the denaturation of DNA progresses as we raise the temperature, but implicitly this plot is generated by increasing the temperature very slowly, so that for each temperature, the system is in equilibrium. What can we say about the kinetics of denaturation and renaturation? We can write the denaturation reaction as

$$\mathrm{DS} \rightarrow 2\ \mathrm{SS}, \tag{1.210}$$

where DS and SS denote double stranded and single stranded DNA molecules. Suppose that we start at a temperature well below $T_{\rm m}$, and suddenly jump to a temperature $T \gg T_{\rm m}$. Now we can follow the UV absorption as a function of time, using this absorption as a measure of the fraction of SS molecules. When we do this, we find that the denaturation occurs very rapidly, and this time course is independent of the concentration of the DNA. This is consistent with what we have learned in Section 1.2, if the reaction in Eq (1.211) really is a first order chemical reaction.

Now let's ask what happens if, having reached equilibrium at $T \gg T_{\rm m}$, we drop the temperature suddenly, to $T \ll T_{\rm m}$. We might expect to see the reaction

$$2\ \mathrm{SS} \rightarrow\ \mathrm{DS}, \tag{1.211}$$

but in fact not much happens at all. Part of the reason is that denatured single strands of DNA easily find weak intramolecular interactions that are stable at low temperatures, and need to be overcome before the renaturation reaction can occur. To have the best chance of observing renaturation in a reasonable amount of time, we should bring the sample from $T \gg T_{\rm m}$ to a temperature just below $T_{\rm m}$, where all bonds other than the "correct" hydrogen bonds between strands are most likely to be broken. When this is done, the renaturation reaction occurs, as one expects from our general discussion of second order kinetics, with a time course that depends on the initial concentration of single stranded DNA.

More precisely, if C is the concentration of single stranded DNA molecules, then from Section 1.2 we know that the reaction in Eq (1.211) should be described by

$$\frac{dC}{dt} = -kC^2, \tag{1.212}$$

where k is the second order rate constant that characterizes this reaction. We recall from Eq (1.95) that the solution to this equation is

$$C(t)/C_0 = \frac{1}{1 + kC_0t}, \tag{1.213}$$

where C_0 is the initial concentration of single stranded DNA. This fits the data from experiments like those shown in Fig 1.22, and makes the important prediction that the time scale of the reaction should be inversely proportional to the initial concentration, and this is easily verified.

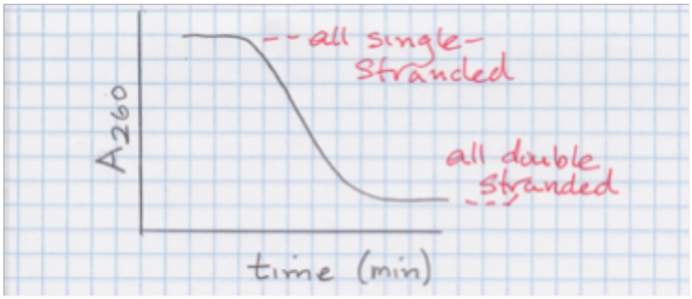


Figure 1.22: Time course of the DNA renaturation reaction. We start at a temperature $T > T_{\rm m}$, and jump to $T < T_{\rm m}$.

To be more quantitative, we need to think about how we defien and measure concentration. For a polymer like DNA, there are two possible definitions:

Definition 1: the number of polymer molecules per unit volume
Definition 2: the number of monomer subunits per unit volume.

Obviously, for DNA molecules containing thousands or millions of nucleotide subunits, these two definitions give very different numbers. Optical methods, such as absorption of UV light depend on concentration of the subunits (it is the bases that absorb the light) and thus the conventional assessment of DNA or RNA concentration is by Definition 2, not Definition 1. Consider a collection of 10^9 large DNA molecules in 1 ml of solution, with average length $10,000$ nucleotides (these molecules are referred to as a 10 kilobase-pair (kb) in length). The total number of bases available to absorb UV light will be $10,000 \times 10^9 \times 2 = 2 \times 10^{13}$ bases. This solution will absorb a readily measureable amount of UV light. If we were to cut the molecules in this solution into pieces of about 1 kb, we would have ten times as many molecules, and thus, by Definition 1 the concentration would change tenfold. But the number of bases would remain the same, and by Definition 2 (and by measurement using UV absorption) the concentration would remain the same.

Nucleic acid biochemists and molecular biologists normally use Definition 2, because that is what we measure. However, in doing molecular manipulations (such as DNA cloning), it is not the size of the molecules that is important, but the number of ends. Consider the simplest of all cloning steps: joining one molecule of DNA to another. In this case, we need to know the concentration of ends, regardless of the size of the individual DNA molecules, i.e. the DNA concentration by Definition 1. Knowing this requires more than what we can learn from UV absorption—we need to know also the sizes of the molecules.

There is also one more complication in analyzing DNA renaturation—but this complication becomes a method for learning something about the DNA molecules themselves. If we take identical DNA molecules, e.g. from a population of bacterial DNA viruses, and denature them, we will get exactly two kinds of single-stranded molecules each of which is the complement of the other. In the following discussion we will call these W (for Watson) and C (for Crick). They have the same information, but different sequences, and their chemical orientation is opposite. Suppose, however, that we were to fragment the DNA into little pieces, and then denature them? This will make things a lot more complicated, because now we have many different kinds of molecules. In Fig 1.23, W is blue, and C is red, and the arrows indicate their relative chemical orientation. Fragmentation will generate a great variety of different double-stranded DNA molecules (a, b, c, d, e, etc.). When these are denatured, there will be twice as many single-stranded molecules in the solution. Some of them are still complementary, but if the number of fragments is large the probability that any two molecules taken at random are complementary becomes extremely small. Specifically, a_{w} can renature and form a double helix only with a_{c} because all the others have different sequences. Yet the whole ensemble of molecules should eventually renature, because each single-stranded fragment has a complement in the solution because of the way it was made. But the process will be slow.

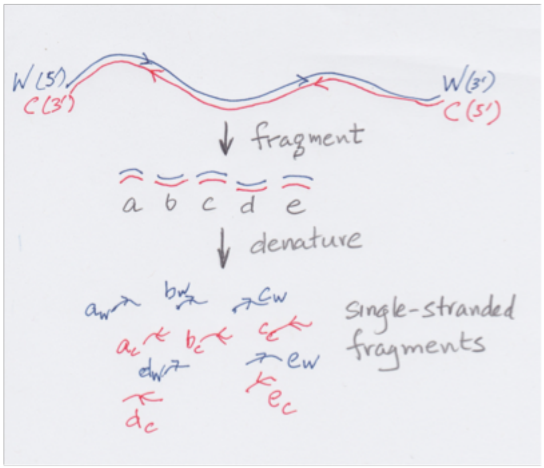


Figure 1.23: Schematic of an experiment in which we fragment and then denature DNA.

But suppose that the original virus contained three copies of the same sequence in its DNA. After fragmentation and denaturation, we would have 3 times as many copies per unit volume of the single stranded molecules a_{w}, a_{c}, b_{w}, b_{c}, etc. and time course of the renaturation reaction would be three times faster. In other words, the sequence complexity matters, and, conversely, it should be possible to infer sequence complexity from the kinetics of renaturation of fragmented and denatured DNA molecules.

In the following examples,[7] we will make use of the single double stranded DNA molecules that comprise the genomes of bacteriophages T4 and T7, both of which are viruses that grow on the common bacterium *Escherichia coli.* Preparations of T4 yield single DNA molecules about 110 kb in length; T7 DNA contains molecules about 40 kb in length. Neither molecule contains repeated sequences, and T4 and T7 are not homologous—they have entirely different nucleotide sequences. We can see the effect of concentration directly if we take just T7 DNA, fragment and denature it, and then renature it at two different concentrations of total DNA (10 μg/ml and 30 μg/ml,

---

[7] Our discussion here follows *Genetics: Analysis of Genes and Genomes, Seventh Edition* D Hartl & E Jones (Joens & Bartlett, Sudbury MA, 2009).

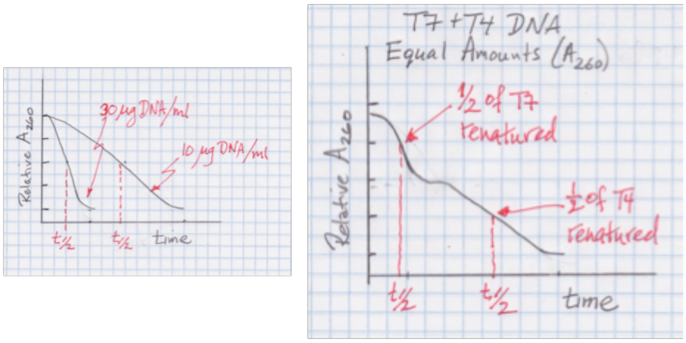


Figure 1.24: At left, renaturation kinetics of T7 DNA, at two different initial concentrations. At right, the corresponding experiment with a mixture of T7 and T4 DNA. The intial concentrations of the two species of DNA are the same, as measured by A_{260}, which means that we have the sme number of *bases* from each species. Because the two genomes are of different lengths, this corresponds to different numbers of single stranded molecules.

measured as A260). As we expect, the higher concentration renatures much faster because if we have N copies of the single-stranded fragments $a_{\rm w}$ and $a_{\rm c}$ at $10\,\mu$g/ml, we will have 3N copies of them at $30\,\mu$g/ml. If we now make a mixture of equal amounts (again determined by A_{260}) of T4 and T7 DNAs, fragmented and denatured, and do a renaturation experiment with them, we find that they behave independently. Indeed, even with this relatively modest difference in sequence complexity (40kb versus 110kb) we can see a very robust separation of the half times for renaturation of the two DNAs; indeed, most of the T7 DNA has renatured before the T4, as predicted.

Formally, sequence complexity is defined as the longest non-repetitive sequence in a genome. For bacteriophages T4 and T7, it is the entire genome (i.e. 110 kb and 40 kb, respectively). For simple sequences like

5'TTTTTTTTTT 5'GCGCGCGCGC 5'AGTAGTAGTAGT
3'AAAAAAAAAA 3'CGCGCGCGCG 3'TCATCATCATCA

the complexity is 1, 2 or 3 basepairs, respectively. Having established above that renaturation kinetics is connected to complexity we can seek to infer

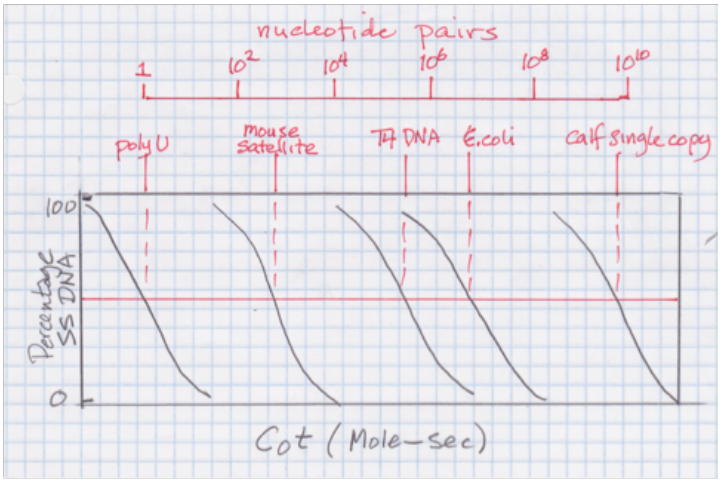


Figure 1.25: C_0t curves for several samples of DNA, comparing with the known number of base pairs in each molecule.

complexity from the kinetics. Equation (1.213) above provides a characteristic quantity $C_0t_{1/2}$ which is equal to the reciprocal of the second-order renaturation constant k. The relationship between $C_0t_{1/2}$ (in units of Molar–sec) and complexity (in nucleotide pairs) can be calibrated experimentally by renaturing fragmented single-stranded naprations derived from double-stranded DNA molecules whose complexity is known by other means. This empirical calibration yields the generalization that under standard renaturation conditions the complexity $N = 5 \times 10^5\, C_0t_{1/2}/(\mathrm{M} \cdot \mathrm{s})$, as in Fig 1.25.

The genomes of many organisms contain repetitive DNA sequences. Notably, mammalian genomes (which are many orders of magnitude larger than the genomes of viruses and bacteria) consist of about equal amounts of single-copy and repetitive DNA sequences. The repeated sequences can be short, meaning that some of these sequences are present in thousands to millions of copies. The numbers and sizes of repeated sequences can readily be estimated from renaturation kinetics: the principle is exactly the same as the example given above of a mixture of T4 and T7 DNAs. The example shown here is typical for higher eukaryotic genomic DNAs: about 20 percent of the total DNA is highly repetitive DNA comprised of low complexity sequences, about 30 percent is middle-repetitive DNA of higher complexity, and about 50% is single-copy, typically with a complexity of about 10^9

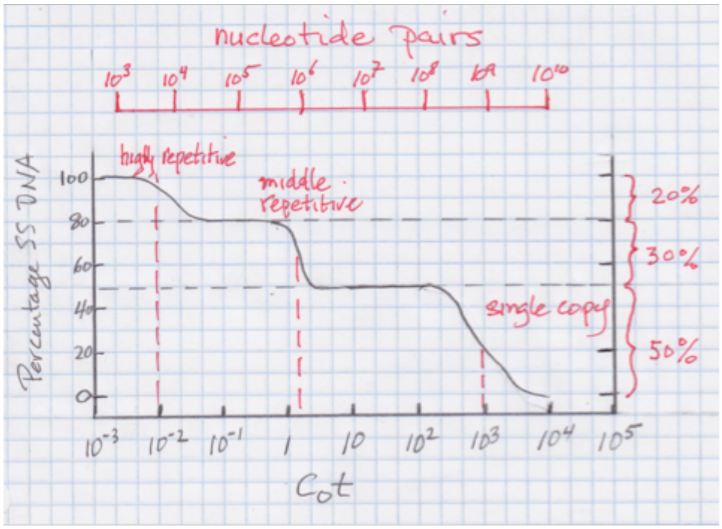


Figure 1.26: Renaturation of DNA fragmented from a complex organism, in which different segements of the DNA sequence are repeated different numbers of times.

nucleotide pairs. Often the repeated sequences are referred to as satellites, because their DNA sequences are sufficiently different from the single-copy DNA to have different physical properties, such as density in CsCl, that allow them to be separated from the bulk of the DNA.

Problem 29: Be sure that you understand Fig 1.26. How repetitive are the "middle repetitive" sequences?

It should be clear that the remarkable intrinsic ability of DNA strands to spontaneously renature by pairing specifically only with strands containing exactly complementary sequences is the essential property of DNA on which all of life is founded. This property also accounts for the kinetics of DNA renaturation. Long before DNA sequencing was possible study of DNA renaturation kinetics not only validated this property, but made possible the measurement of the sequence complexity and composition of our genomes.

Problem 30: The total genomic DNA of a newly-discovered species of newt contains 1200 copies of a 2 kb repeated sequence, 300 copies of a 6 kb repeated sequence as well as 3000 kb of single-copy DNA.

(a.) What will the "Cot curve" (i.e. plot of the fraction of DNA remaining single-stranded vs. C_0t) look like? Be sure to label the axes, and indicate the fractional contribution of the different kinds of DNA.

(b.) Devise a procedure to prepare reasonably pure samples of the three kinds of DNA. Explain how you would calculate the times of annealing required for each step.

Chapter 2

Resonance and response

In this section of the course we begin with a very simple system—a mass hanging from a spring—and see how some remarkable ideas emerge. We will see, for example, that it is useful to use imaginary numbers to describe real things. Most importantly, we will understand how to describe the way systems respond to small perturbations, and this turns out to be very general. Following this path, our intuitive notions that something is stable or unstable can be given precise mathematical formulations. We will take all of this far enough to see how the ideas can be used in describing complex biological phenomena, from the switches that control the expression of genes to the electrical impulses that carry information throughout the brain.

2.1 The simple harmonic oscillator

We have been talking about mechanics problems in which there is (a) no force, (b) a constant force, or (c) a force proportional to the velocity. The other "simple" case is when the force is proportional to the position, as is the case when we stretch a spring. Notice that we do these simple cases not because we want to torture you with simplified problems that are irrelevant in nature, but rather because, from our discussion of Taylor series and "laws" like Hooke's law or Ohm's law, we know that these simple cases are the leading approximations to more complex situations. Hopefully this will be clear before too long.

So, let us consider, as in Fig 2.1, a mass M hanging at the end of a spring with stiffness κ; you can imagine either that the system lies on its side, or that we ignore the force of gravity. If we measure the position x of

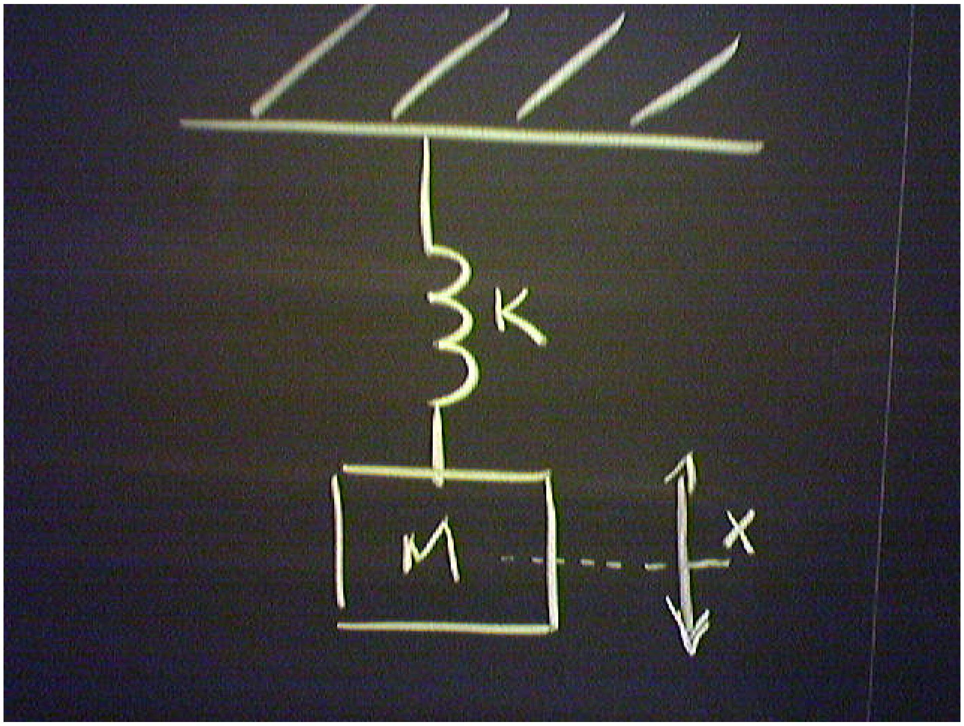


Figure 2.1: A mass M bound by a spring of stiffness κ, as in Eq (2.2).

the spring in coordinates such that the equilibrium position is $x = 0$,[1] then the force on the mass is

$$F = -\kappa x. \tag{2.1}$$

In this problem $F = ma$ therefore corresponds to the differential equation

$$M\frac{d^2x(t)}{dt^2} = -\kappa x(t). \tag{2.2}$$

This is an example of a system usually called a *simple harmonic oscillator*, for reasons that I hope will become clear as we go along.

We will see, remarkably, that to give a full solution it is natural to write the real displacement of the mass in terms of complex numbers. Once we understand how to do this we will see that we can generate a rather complete

---

[1] You should convince yourself that we can include gravity just by redefining the zero point on the x axis.

view of the problem. It is important that the seemingly special problem of the harmonic oscillator comes up in many different guises.

Take a moment to think about what Eq (2.2) means. We can draw the function $x(t)$. At every point on the graph we can compute the local slope (the derivative or velocity) and then from this new graph we can compute the local slope again (the acceleration). Up to constants, Eq. (2.2) is telling us that this function we obtain by differentiating twice is just the negative of the original function $x(t)$—if we graph the second derivative and flip it upside down it should overly the original graph. Obviously not all functions have this property, and indeed you will learn in your math courses the very important theorem that (once we specify the initial conditions) the functions which satisfy differential equations are unique. This is crucial because it means that if we find *a* solution of a differential equation that satisfies all the initial conditions, even if we have to guess the form of the solution, then we're done, because there can't be any other solutions.

Equation (2.2) has a very simple form. Notice that there are two derivatives, so we say it is a second order equation. Further, the equation is linear, which means all the terms are proportional to x. The fact that equation is linear implies that the sum of two solutions is also a solution. This is a subtle idea, and we will come back to it. Finally, all the coefficients which appear in the equation are constants, with no explicit dependence on time. While we may not know how to solve all differential equations, we'll make a lot of progress on this important special class.

As noted previously, the best way to solve a differential equation is to ask someone who knows the answer. In this case, *you* know the answer from your calculus course. Recall that

$$\begin{aligned} \frac{d}{dt}\sin(\omega t) &= \omega\cos(\omega t) && (2.3) \\ \frac{d}{dt}\cos(\omega t) &= -\omega\sin(\omega t). && (2.4) \end{aligned}$$

Then if we take two derivatives we have

$$\begin{aligned} \frac{d^2}{dt}\sin(\omega t) &= \frac{d}{dt}[\omega\cos(\omega t)] = -\omega^2\sin(\omega t) && (2.5) \\ \frac{d^2}{dt}\cos(\omega t) &= \frac{d}{dt}[-\omega\sin(\omega t)] = -\omega^2\cos(\omega t). && (2.6) \end{aligned}$$

Thus, sine and cosine have the properties of the function that we are looking for: when you differentiate twice, you get back something proportional to the function itself, with a minus sign.

To be more explicit, let's rewrite Eq (2.2), dividing through by the mass:

$$\frac{d^2x(t)}{dt^2} = -\left(\frac{\kappa}{M}\right)x(t). \tag{2.7}$$

Then we also have

$$\frac{d^2\sin(\omega t)}{dt^2} = -\omega^2\sin(\omega t), \tag{2.8}$$

which means that $x(t) = \sin(\omega t)$ is a solution to the equation, provided that we identify

$$\omega^2 = \kappa/M. \tag{2.9}$$

For the same reasons, $x(t) = \cos(\omega t)$ is also a solution, with the same value of ω.

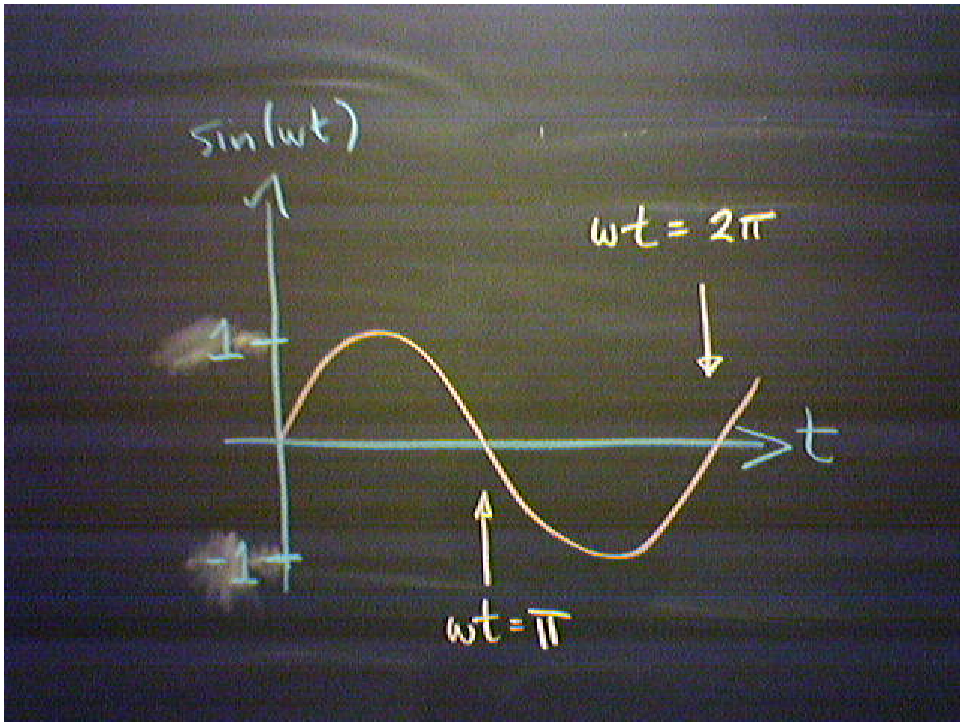


Figure 2.2: The function $\sin(\omega t)$.

Before proceeding it is worth remembering a few facts about sines and cosines. As shown in Fig 2.2, the sine function oscillates between +1 and

-1; when the time t shifts by an amount T such that $\omega T = 2\pi$, the function has the same value. We say that $T = 2\pi/\omega$ is the period of the oscillation and $f = 1/T = \omega/2\pi$ is the frequency. Sometimes we are sloppy and refer to ω as the frequency.

Problem 31: When a 50 kg person sits on top of a car, the car body moves down toward the ground by 3 inches. The car body itself weighs one ton.

(a.) What is the effective stiffness of the spring which supports the weight of the car? Use some useful set of units!

(b.) The stiffness comes from the shock absorbers. Suppose that there is no viscosity or damping in the shocks. Then if you are sitting on top of the car and suddenly jump off, the height of the car body should oscillate. What is the oscillation frequency?

What we have found is that $x(t) = \sin(\omega t)$ is "a solution" of the differential equation that encapsulates $F = ma$ for this system, and we have also found that $x(t) = \cos(\omega t)$ is "a solution." But have we found "the solution"? What do we mean by this? Why is there more than one solution?

Let's step back from the particular equations and think more generally. As emphasized by Laplace, Newtonian mechanics presents us with a dramatic view of the world in which, given the initial conditions, we can solve the differential equations describing the motion of all the relevant objects and hence predict the future with, it would seem, complete certainty. Obviously this depends on the differential equations having unique solutions—if we claim to be able to predict the trajectory of a falling object starting with $F = ma$, then this equation had better have a unique solution once we specify all the initial conditions. If the solutions weren't unique, then maybe each time we drop a ball something different would happen (!).

So the correct statement is that solutions of the differential equations are unique *once we specify all the initial conditions.* How many initial conditions are there? We saw in simple cases that we needed to specify the initial position and the initial velocity in order to integrate the equations of motion, and this is quite general. So when we talk about "a solution" we mean a solution that is consistent with *some* set of initial conditions; "the solution" means the solution consistent with the initial conditions in our particular physical setting.

What we might be able to do, and indeed what we might hope to do, is to write down a solution that has parameters, and show that by setting these parameters we can be consistent with any set of initial conditions. Then what we really have is a family of solutions, and at this point we really are done with our problem—we have a whole family of functions $x(t)$, each of which solves the differential equation, and by picking the right member of this family we can agree with the initial position and velocity of the particle.

You have already seen this idea of *families of solutions* in the simplest case of zero force. Recall that in this case the position as a function of time is given by $x(t) = x(0) + v(0)t$. This function describes a straight line when we plot x vs t, but this straight line can have any slope [depending on $v(0)$] and any intercept [depending on $x(0)$)]. So really we have a family of lines, all of which solve the differential equation $F = ma$, but to pick one of them we need to know the initial position and initial velocity of the particle.

Our example of the mass on a spring is a little more complicated than the case of zero force, but again simpler than it could be. The simplicity here is that the equation is *linear*. That is, if we look at the terms in

$$\frac{d^2x(t)}{dt^2} = -\left(\frac{\kappa}{M}\right)x(t), \tag{2.10}$$

we see that both terms are proportional to x, and this is what we mean by linearity. There is a special consequence of linearity, and this is the *superposition* of solutions. Suppose that we have found one solution of our equation, a solution consistent with one set of initial conditions, and let's call this solution $x_1(t)$. Suppose also that we have found another solution, consistent with a different set of initial conditions, and let's call this $x_2(t)$. What is remarkable about linear equations is that now we can construct another function, $x(t) = Ax_1(t) + Bx_2(t)$, and this is also a solution, one which matches yet a third set of initial conditions. To see this, we can just check by substitution:

$$\begin{aligned}
\frac{d^2x(t)}{dt^2} &= \frac{d^2[Ax_1(t) + Bx_2(t)]}{dt^2} && (2.11)\\
&= A\frac{d^2x_1(t)}{dt^2} + B\frac{d^2x_2(t)}{dt^2} && (2.12)\\
&= -\left(\frac{\kappa}{M}\right)Ax_1(t) - \left(\frac{\kappa}{M}\right)Bx_2(t) && (2.13)\\
&= -\left(\frac{\kappa}{M}\right)[Ax_1(t) + Bx_2(t)] && (2.14)\\
&= -\left(\frac{\kappa}{M}\right)x(t), && (2.15)
\end{aligned}$$

where in going from Eq (2.12) to (2.13) we use the fact that $x_1(t)$ and $x_2(t)$ each are solutions, which means that $d^2x_1(t)/dt^2 = -(\kappa/M)x_1(t)$, and similarly for $x_2(t)$. Thus we see that we can use these two solutions to construct a whole family of new solutions just by linear combination. Notice that this argument doesn't depend on knowing the exact form of the solutions, since all we use is the linearity of the equation.

Why is this so important? By combining two solutions we generate a whole family of solutions, but these have two parameters, A and B. But we know that once we match the initial position and initial velocity, the solution is unique. Thus if we can adjust A and B to match the initial position and velocity, we are done: We have constructed the whole family of solutions that we need.

Let's see how this plays out with our particular example. We have seen that one possible solution to our problem is $x_1(t) = \sin(\omega t)$, and another is $x_2(t) = \cos(\omega t)$. Thus we can construct the linear combination

$$x(t) = A\sin(\omega t) + B\cos(\omega t), \tag{2.16}$$

and this should also be a solution. Now because $\sin(0) = 0$ and $\cos(0) = 1$, we can see that

$$x(0) = B. \tag{2.17}$$

If we differentiate to find the velocity,

$$\begin{aligned} v(t) &\equiv \frac{dx(t)}{dt} = \frac{d[A\sin(\omega t) + B\cos(\omega t)]}{dt} && (2.18)\\ &= A\omega\cos(\omega t) - B\omega\sin(\omega t), && (2.19)\end{aligned}$$

so that

$$v(0) = A\omega. \tag{2.20}$$

So in this case the relationship between the coefficients A, B and the initial conditions is quite simple:

$$\begin{aligned} A &= x(0), && (2.21)\\ B &= \frac{v(0)}{\omega}. && (2.22)\end{aligned}$$

Let's summarize what we have done:

- The differential equation $F = ma$ that describes a mass M hanging from a spring of stiffness κ is

  $$M\frac{d^2x(t)}{dt^2} = -\kappa x(t). \tag{2.23}$$

- Solutions to this equation include

  $$\begin{aligned} x_1(t) &= \sin(\omega t), \text{ and} && (2.24) \\ x_2(t) &= \cos(\omega t), && (2.25) \end{aligned}$$

  where we have to choose

  $$\omega = \sqrt{\frac{\kappa}{M}}. \qquad (2.26)$$

- Because Eq (2.23) is linear, we can combine these solutions to form a family of solutions

  $$x(t) = A\sin(\omega t) + B\cos(\omega t). \qquad (2.27)$$

- Finally, we can adjust the constants A and B to match the initial position and initial velocity:

  $$x(t) = \frac{v(0)}{\omega}\sin(\omega t) + x(0)\cos(\omega t). \qquad (2.28)$$

You might want to play with this solution a little bit, plotting it and seeing what it looks like. We will come back and do this, but first let's look at a very different way of finding these solutions, one which is much more general.

Problem 32: Show that you can rewrite Eq (2.28) in the form

$$x(t) = A\cos(\omega t + \phi), \qquad (2.29)$$

where A is called the amplitude and ϕ is called the phase of the oscillation. Draw (by hand, not with the computer!) the function $x(t)$, being careful to show units on both axes and marking the point where $t = 0$. Indicate the features of the graph that correspond to the amplitude, phase and frequency.

Recall our (only partly) joking idea that there are three ways to solve a differential equation. What we did last time was to ask someone who knew the answer—you knew the properties of sine and cosine from your calculus course, and you could see that this is what you needed to solve the equation. But you remember that when we looked at a mass moving through a fluid, or first order chemical kinetics, we also encountered linear differential equations with constant coefficients. The simplest equation in this class of interest is of the form

$$\frac{dx(t)}{dt} = ax(t), \tag{2.30}$$

where a is a constant. We found that we could solve this by guessing a solution of the form $x(t) = Ae^{\lambda t}$, and then everything works if we set $\lambda = a$ and $A = x(0)$. Can we use this same "guess and check" method (the second of the three methods) to solve the mass–spring problem?

To get started, suppose that we have a second order differential equation which I'll write in the suggestive form

$$\frac{d^2x}{dt^2} = a^2x. \tag{2.31}$$

You can see that $x(t) = Ae^{at}$ still is a solution. In fact, the exponential function has the property that differentiating is just multiplication by a constant:

$$\begin{align}
\frac{d}{dt}\exp(\lambda t) &= \lambda\exp(\lambda t) \tag{2.32}\\
\frac{d^2}{dt^2}\exp(\lambda t) &= \lambda^2\exp(\lambda t) \tag{2.33}\\
&\cdots \tag{2.34}\\
\frac{d^n}{dt^n}\exp(\lambda t) &= \lambda^n\exp(\lambda t). \tag{2.35}
\end{align}$$

Thus if we try to solve Eq. (2.31) by *guessing* a solution of the form $x(t) \propto \exp(\lambda t)$, we see that this will work if (and only if)

$$\lambda^2 = a^2, \tag{2.36}$$

which means that $\lambda = \pm a$. Now we use the idea of combining solutions to generate a whole family:

$$x(t) = A\exp(at) + B\exp(-at), \tag{2.37}$$

and we have to set the two constants A and B by fixing the initial position and initial velocity as in the discussion above. Again there are two arbitrary constants because we are looking at a second order equation.

All this is fine, but how do we use it to solve the equation we really are interested in, for the mass on a spring? As before we can write this as

$$\frac{d^2x(t)}{dt^2} = \left[-\frac{\kappa}{M}\right]x(t). \tag{2.38}$$

This is just like Eq. (2.31) if we identify $a^2 = -\kappa/M$. To put it another way, we can try to solve Eq. (2.38) by guessing that $x(t) = A\exp(\lambda t)$, and if we substitute we find

$$\begin{aligned}
\frac{d^2}{dt^2}A\exp(\lambda t) &= \left[-\frac{\kappa}{M}\right]A\exp(\lambda t) && (2.39)\\
A\lambda^2\exp(\lambda t) &= \left[-\frac{\kappa}{M}\right]A\exp(\lambda t) && (2.40)\\
\lambda^2 &= \left[-\frac{\kappa}{M}\right] && (2.41)\\
\lambda^2 + \frac{\kappa}{M} &= 0. && (2.42)
\end{aligned}$$

Thus we see that λ obeys a quadratic equation, although a very simple one in this case. There are two solutions, and this is related to the fact that this is a second order equation:

$$\lambda = \pm\sqrt{-\frac{\kappa}{M}}. \tag{2.43}$$

Now we see something strange, namely that our solution is the square root of a negative number.

For most of you, at some early point in your education you were taught about square roots, and your teachers explained that you can't take the square root of a negative number. Then at some point in high school, perhaps, they told you that it's OK, but it gets a special name: $i = \sqrt{-1}$ is the unit imaginary number. So, we have the result that the solution of $F = ma$ for this problem must be of the form

$$x(t) = A\exp(+i\omega t) + B\exp(-i\omega t). \tag{2.44}$$

It's absolutely fantastic that imaginary numbers appear in the solution to a physics problem.

2.2 Magic with complex exponentials

We don't really know what aspects of complex variables you learned about in high school, so the goal here is to start more or less from scratch. Feedback will help us to help you, so let us know what you do and don't understand. Also, if something is not immediately clear you should work through examples ... as usual.

The introduction to square roots in school often makes the point that the square root of a negative number is not defined, since after all when we square a number we always get something positive. Then at some point you are told about imaginary numbers, where the basic object is $i = \sqrt{-1}$. It is not clear, perhaps, whether this is some sort of joke (calling them "imaginary" probably doesn't help!). Here we are asking you to take these things very seriously.

Figure 2.3: From our local cafe.

Remember that when you first learned about negative numbers (a long time ago ...) there was some mystery about what you do when you add, multiply, etc.. In the end the answer is that the rules are the same, and you have to apply them in a consistent way. This is true also for complex or imaginary numbers.

We begin by recalling that with x and y real numbers, we can form the complex number $z = x + iy$. The object i is the square root of negative one, $i = \sqrt{-1}$. Then if we have two of these numbers

$$\begin{aligned} z_1 &= x_1 + iy_1 && (2.45) \\ z_2 &= x_2 + iy_2 && (2.46) \end{aligned}$$

we can go through all the usual operations of arithmetic:

$$\begin{aligned} z_1 + z_2 &\equiv (x_1 + iy_1) + (x_2 + iy_2) && (2.47) \\ &= (x_1 + x_2) + i(y_1 + y_2); && (2.48) \\ z_1 - z_2 &\equiv (x_1 + iy_1) - (x_2 + iy_2) && (2.49) \\ &= (x_1 - x_2) + i(y_1 - y_2); && (2.50) \\ (z_1) \times (z_2) &\equiv (x_1 + iy_1) \times (x_2 + iy_2) && (2.51) \\ &= x_1x_2 + x_1(iy_2) + iy_1x_2 + iy_1(iy_2) && (2.52) \\ &= x_1x_2 + i(x_1y_2 + x_2y_1) + (i^2)y_1y_2 && (2.53) \\ &= x_1x_2 + i(x_1y_2 + x_2y_1) - y_1y_2 && (2.54) \\ &= x_1x_2 - y_1y_2 + i(x_1y_2 + x_2y_1), && (2.55) \end{aligned}$$

where in the second to last step we use the fact that $i^2 = -1$. Note that this list leaves out division, which we'll get back to in a moment.

One very useful operation that is new for complex numbers is called "taking the complex conjugate," or "complex conjugation." For every complex number $z = x + iy$, the complex conjugate is *defined* to be $z^* = x - iy$. Note that in elementary physics we usually use z^* to denote the complex conjugate of z; in the math department and in some more sophisticated physics problems it is conventional to write the complex conjugate of z as $\bar{z}$, but of course this is just notation. The crucial fact is that

$$\begin{aligned} z \times z^* &\equiv (x + iy) \times (x - iy) && (2.56) \\ &= x^2 + x(-iy) + iyx + (i)(-i)y^2 && (2.57) \\ &= x^2 + i(-xy + yx) - (i^2)y^2 && (2.58) \\ &= x^2 + y^2. && (2.59) \end{aligned}$$

Often we write $zz^* = |z|^2$, just the way we write the length of a vector in terms of its dot product with itself, $\vec{x}\cdot\vec{x} = |\vec{x}|^2$. This is an important thing on its own, as we will see, but also it makes division a lot easier, which we do now.

There is a trick, which is to clear the complex numbers from the denominator any time we divide:

$$\begin{aligned}
\frac{z_1}{z_2} &\equiv \frac{(x_1 + iy_1)}{(x_2 + iy_2)} && (2.60)\\
&= \frac{z_1}{z_2} \cdot \frac{z_2^*}{z_2^*} && (2.61)\\
&= \frac{z_1 z_2^*}{z_2 z_2^*} && (2.62)\\
&= \frac{z_1 z_2^*}{|z_2|^2} && (2.63)\\
&= \frac{(x_1 x_2 + y_1 y_2) + i(y_1 x_2 - x_1 y_2)}{x_2^2 + y_2^2} && (2.64)
\end{aligned}$$

Problem 33: You should be able to add, subtract, multiply and divide these pairs of complex numbers: (a) $z_1 = 3+4i$, $z_2 = 4+3i$. (b) $z_1 = 3+4i$, $z_2 = 4-3i$. (c) $z_1 = 7-9i$, $z_2 = 27 + 12i$. And you should be able to make up your own examples!

It is useful to think about a complex number as being a vector in a two dimensional space, as in Fig. 2.4. In this view, the x axis is the real part

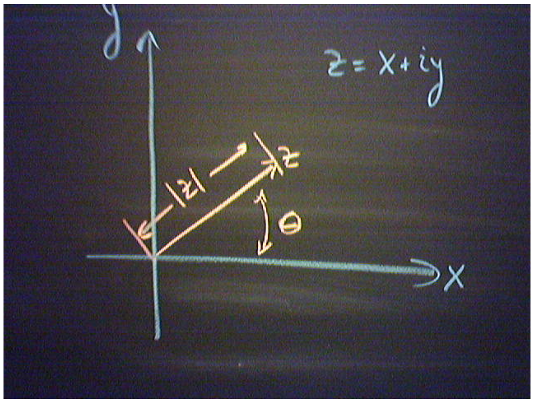


Figure 2.4: Thinking of a complex number $z = x+iy$ as a vector in the $x-y$ plane. This is often called the “complex plane.”

and the y axis is the imaginary part, as is hinted when we write $z = x + iy$. The length of the vector is

$$|z| \equiv \sqrt{x^2 + y^2} = \sqrt{|z|^2} = \sqrt{zz^*}, \tag{2.65}$$

and the angle that this makes with the x axis is given by

$$\theta = \tan^{-1}\left(\frac{y}{x}\right). \tag{2.66}$$

In this notation,

$$\begin{aligned} z &\equiv x + iy && (2.67) \\ &= \sqrt{x^2 + y^2}\left(\frac{x}{\sqrt{x^2 + y^2}} + i\frac{y}{\sqrt{x^2 + y^2}}\right) && (2.68) \\ &= |z|(\cos\theta + i\sin\theta). && (2.69) \end{aligned}$$

Now there is a very pretty thing, which is that if we multiply two complex numbers, the magnitudes get multiplied and the angles just add:

$$\begin{aligned} z_1 \times z_2 &\equiv |z_1|(\cos\theta_1 + i\sin\theta_1) \times |z_1|(\cos\theta_1 + i\sin\theta_1) && (2.70) \\ &= (|z_1||z_2|)[(\cos\theta_1\cos\theta_2 - \sin\theta_1\sin\theta_2) \\ &\quad + i(\sin\theta_1\cos\theta_2 + \sin\theta_1\cos\theta_1)] && (2.71) \\ &= (|z_1||z_2|)[\cos(\theta_1 + \theta_2) + i\sin(\theta_1 + \theta_2)], && (2.72) \end{aligned}$$

where in the last step we use the trigonometric identities

$$\begin{aligned} \cos(\theta_1 + \theta_2) &= \cos\theta_1\cos\theta_2 - \sin\theta_1\sin\theta_2 && (2.73) \\ \sin(\theta_1 + \theta_2) &= \sin\theta_1\cos\theta_2 + \sin\theta_1\cos\theta_1. && (2.74) \end{aligned}$$

By the same reasoning, one finds

$$\frac{z_1}{z_2} = \frac{|z_1|}{|z_2|}[\cos(\theta_1 - \theta_2) + i\sin(\theta_1 - \theta_2)]. \tag{2.75}$$

Problem 34: Derive Eq (2.75). Also, in terms of these θ_1 and θ_2, what is the condition for multiplying two complex numbers and getting a real answer?

We now have enough tools to figure out what we mean by the exponential of a complex number. Specifically, let's ask what we mean by $e^{i\phi}$. This is a complex number, but it's also an exponential and so it has to obey all the rules for the exponentials. In particular,

$$\begin{aligned} e^{i\phi_1}e^{i\phi_2} &= e^{i(\phi_1+\phi_2)} && (2.76)\\ \frac{e^{i\phi_1}}{e^{i\phi_2}} &= e^{i(\phi_1-\phi_2)}. && (2.77)\end{aligned}$$

You see that the variable ϕ behaves just like the angle θ in the geometrial representation of complex numbers. Furthermore, if we take the complex number $z = e^{i\phi}$ and multiply by its complex conjugate ...

$$e^{i\phi} \times \left[e^{i\phi}\right]^* = e^{i\phi} \times \left[e^{-i\phi}\right] = e^{i(\phi-\phi)} = 1. \qquad (2.78)$$

Thus $z = e^{i\phi}$ is a complex number with unit magnitude, and the angle in the complex plane is just ϕ itself. Thus we see that

$$e^{i\phi} = \cos\phi + i\sin\phi, \qquad (2.79)$$

which finally tells us what we mean by the complex exponential. Notice that something like this formula had to be true because we know that the solution to the differential equation for the harmonic oscillator can be written either in terms of sines and cosines or in terms of complex exponentials; since solutions are unique, these must be ralted to each other.

If you consider the special case of $\phi = \pi$, then $\sin\phi = 0$ and $\cos\phi = -1$, leading to the famous Euler formula

$$e^{i\pi} + 1 = 0. \qquad (2.80)$$

This is a really beautiful equation, linking the mysterious transcendental numbers e and π with the imaginary numbers.

Problem 35: Derive the sum and difference angle identities by multiplying and dividing the complex exponentials. Use the same trick to derive an expression for $\cos(3\theta)$ in terms of $\sin\theta$ and $\cos\theta$.

Armed with these tools, let's get back to our (complex) expression for the trajectory,

$$x(t) = A\exp(+i\omega t) + B\exp(-i\omega t).$$

We now know that

$$\exp(\pm i\omega t) = \cos(\omega t) \pm i\sin(\omega t), \tag{2.81}$$

so at least it's clear what our expression means.

To really solve the problem we need to match the initial conditions. We can see that

$$\begin{aligned} x(0) &= A\exp(i\omega\cdot 0) + B\exp(-i\omega\cdot 0) && (2.82)\\ &= A + B, && (2.83)\end{aligned}$$

because $e^0 = 1$, as always. Now in principle A and B are complex numbers,

$$\begin{aligned} A &= \mathrm{Re}A + i\mathrm{Im}A && (2.84)\\ B &= \mathrm{Re}B + i\mathrm{Im}B, && (2.85)\end{aligned}$$

while of course $x(0)$ is the actual position of an object and thus has to be a real number. Let's substitute and see how this works:

$$\begin{aligned} x(0) &= A + B \\ &= \mathrm{Re}A + i\mathrm{Im}A + \mathrm{Re}B + i\mathrm{Im}B && (2.86)\\ &= (\mathrm{Re}A + \mathrm{Re}B) + i(\mathrm{Im}A + \mathrm{Im}B). && (2.87)\end{aligned}$$

So we can match the reality of the initial condition (never mind its value!) only if

$$\mathrm{Im}B = -\mathrm{Im}A. \tag{2.88}$$

Now we need to do the same thing for the initial velocity. By differentiating we see that

$$v(t) \equiv \frac{dx(t)}{dt} = A\frac{de^{i\omega t}}{dt} + B\frac{de^{-i\omega t}}{dt} = A(i\omega)e^{i\omega t} + B(-i\omega)e^{-i\omega t}, \tag{2.89}$$

and hence

$$v(0) = i\omega(A - B). \tag{2.90}$$

Substituting once again,

$$\begin{aligned} v(0) &= i\omega(A-B) \\ &= i\omega(\mathrm{Re}A + i\mathrm{Im}A - \mathrm{Re}B - i\mathrm{Im}B) \qquad (2.91) \\ &= i\omega(\mathrm{Re}A\mathrm{Re}B) + (i)(i\omega)(\mathrm{Im}A - \mathrm{Im}B) \qquad (2.92) \\ &= -\omega(\mathrm{Im}A - \mathrm{Im}B) + i\omega(\mathrm{Re}A - \mathrm{Re}B). \qquad (2.93) \end{aligned}$$

Notice that the real part of the velocity actually comes from the imaginary parts of A and B. In order that the imaginary part of the velocity cancel must have

$$\mathrm{Re}A = \mathrm{Re}B. \qquad (2.94)$$

Thus there really is only one independent complex number here, since we have shown that

This might getting a bit pedantic. Feedback is appreciated.

$$\begin{aligned} A &= \mathrm{Re}A + i\mathrm{Im}A \qquad (2.95) \\ B &= \mathrm{Re}A - i\mathrm{Im}A. \qquad (2.96) \end{aligned}$$

When two complex numbers have this relationship—equal real parts and opposite imaginary parts—we say that they are complex conjugates, and the notation for this is $B = A^*$. The operation * simply replaces i by $-i$ in a complex number, and clearly $(z^*)^* = z$. Hence we can write our solution

$$\begin{aligned} x(t) &= A\exp(+i\omega t) + B\exp(-i\omega t) \\ &= A\exp(+i\omega t) + A^*\exp(-i\omega t). \qquad (2.97) \end{aligned}$$

But note that $\exp(-i\omega t) = [\exp(+i\omega t)]^*$, so we can write

$$\begin{aligned} x(t) &= A\exp(+i\omega t) + A^*[\exp(+i\omega t)]^* \qquad (2.98) \\ &= A\exp(+i\omega t) + [A\exp(+i\omega t)]^*. \qquad (2.99) \end{aligned}$$

Now $x(t)$ is the sum of a complex number and its complex conjugate. But when we add a complex number to its complex conjugate, we cancel the imaginary part and double the real part:

$$\begin{aligned} z + z^* &= [\mathrm{Re}(z) + i\mathrm{Im}(z)] + [\mathrm{Re}(z) - i\mathrm{Im}(z)] \qquad (2.100) \\ &= 2\mathrm{Re}(z). \qquad (2.101) \end{aligned}$$

Thus $x(t)$, according to Eq (2.99) will be real at all times. This is good, of course (!). Interestingly, we didn't actually use this condition—all we did was to be sure that we match the initial conditions, which of course are real. This is sufficient to insure that trajectories are real forever, which is nice.

To proceed further, we recall that all complex numbers can be written as

$$\begin{aligned} z &= \mathrm{Re}z + i\mathrm{Im}z && (2.102)\\ &= |z|(\cos\phi + i\sin\phi) && (2.103)\\ &= |z|\exp(i\phi), && (2.104)\end{aligned}$$

where z is the magnitude of the complex number and ϕ is its phase,

$$\begin{aligned} |z| &= \sqrt{[\mathrm{Re}(z)]^2 + [\mathrm{Im}(z)]^2} && (2.105)\\ \phi &= \tan^{-1}\left[\frac{\mathrm{Im}(z)}{\mathrm{Re}(z)}\right]. && (2.106)\end{aligned}$$

If we do this rewriting of A,

$$A = |A|\exp(i\phi_A), \qquad (2.107)$$

then the trajectory becomes

$$\begin{aligned} x(t) &= [|A|\exp(i\phi_A)\exp(+i\omega t)] + [|A|\exp(i\phi_A)\exp(+i\omega t)]^* && (2.108)\\ &= [|A|\exp(+i\omega t + i\phi_A)] + [|A|\exp(+i\omega t + i\phi_A)]^*. && (2.109)\end{aligned}$$

Thus

$$\begin{aligned} x(t) &= [|A|\exp(+i\omega t + i\phi_A)] + [|A|\exp(+i\omega t + i\phi_A)]^* \\ &= 2\mathrm{Re}[|A|\exp(+i\omega t + i\phi_A)] && (2.110)\\ &= 2|A|\mathrm{Re}[\exp(+i\omega t + i\phi_A)] && (2.111)\\ &= 2|A|\cos(\omega t + \phi_A). && (2.112)\end{aligned}$$

So, we are done, except that we have to connect this solution to the initial conditions.

We want to find the arbitrary parameters $|A|$ and ϕ_A in terms of the initial position and initial velocity. Let's just calculate:

$$\begin{aligned}
x(t=0) &= 2|A|\cos(\omega(0)+\phi_A) && (2.113)\\
&= 2|A|\cos\phi_A && (2.114)\\
v(t=0) &= \left.\frac{dx(t)}{dt}\right|_{t=0} && (2.115)\\
&= \left.\frac{d}{dt}\left[2|A|\cos(\omega t+\phi_A)\right]\right|_{t=0} && (2.116)\\
&= \left.-2|A|\omega\sin(\omega t+\phi_A)\right|_{t=0} && (2.117)\\
v(t=0) &= -2|A|\omega\sin\phi_A && (2.118)\\
\frac{v(t=0)}{\omega} &= -2|A|\sin\phi_A. && (2.119)
\end{aligned}$$

So we have two equations, Eq's (2.114) and (2.119), that link our parameters to the initial conditions. To solve these equations, note that if we sum the square of the two equations we have

$$\begin{aligned}
[x(0)]^2+\left[\frac{v(0)}{\omega}\right]^2 &= (2|A|)^2\cos^2\phi_A+(2|A|)^2\sin^2\phi_A && (2.120)\\
&= (2|A|)^2, && (2.121)
\end{aligned}$$

so that

$$2|A|=\sqrt{[x(0)]^2+\left[\frac{v(0)}{\omega}\right]^2}. \qquad (2.122)$$

Similarly, if we take Eq (2.119) and divide by Eq (2.114), we find

$$\begin{aligned}
\frac{v(0)}{\omega x(0)} &= -\frac{2|A|\sin\phi_A}{2|A|\cos\phi_A} && (2.123)\\
&= \tan\phi_A, && (2.124)
\end{aligned}$$

and hence

$$\phi_A=\tan^{-1}\left[\frac{v(0)}{\omega x(0)}\right]. \qquad (2.125)$$

Thus the amplitude $|A|$ of the oscillation is related to the initial position, with an extra contribution from the initial velocity, while the phase depends

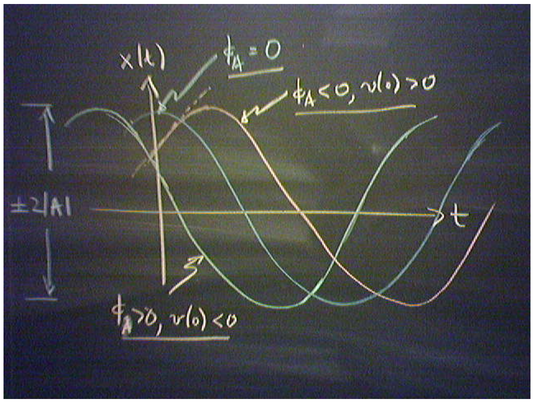


Figure 2.5: Position as a function of time for the harmonic oscillator, from Eq (2.112). Note that when the initial velocity is zero the phase ϕ_A also is zero. Positive initial velocities correspond (in this notation) to negative phases, and vice versa.

on the relative magnitudes of the initial velocity and position. This is shown schematically in Fig 2.5.

Problem 36: Consider the carbon monoxide molecule CO. To a good approximation, the bond between the atoms acts like a Hooke's law spring of stiffness κ and equilibrium length ℓ_0. For the purposes of this problem, neglect rotations of the molecule, so that motion is only in one dimension, parallel to the bond.

(a.) Write the differential equations corresponding to $F = ma$ for the positions x_C and x_O of the two atoms. Remember that the two atoms have different masses m_C and m_O.

(b.) Look for oscillating solutions of the form

$$x_C(t) = x_C^0 + A\exp(-i\omega t) \tag{2.126}$$

$$x_O(t) = x_O^0 + B\exp(-i\omega t), \tag{2.127}$$

where the resting positions x_c^0 and x_O^0 are chosen to match the equilibrium length of the bond. Show that solutions of this form exist, and find the natural frequency ω for these oscillations.

2.3 Damping, phases and all that

If we imagine taking our idealized mass on a spring and dunking it in water (or, more dramatically, in molasses), then there will be a viscous friction or drag force which opposes the motion and is proportional to the velocity:[2]

$$M\frac{d^2x(t)}{dt^2} = -\kappa x(t) - \gamma\frac{dx(t)}{dt}, \tag{2.128}$$

where κ is the spring constant as before and γ is the damping constant. The convention is to put all of these terms on one side of the equation,

$$M\frac{d^2x(t)}{dt^2} + \gamma\frac{dx(t)}{dt} + \kappa x(t) = 0. \tag{2.129}$$

We're going to solve this using our trick of guessing a solution with the form $x(t) = A\exp(\lambda t)$. Recall that

$$\begin{aligned} x(t) &= Ae^{\lambda t} && (2.130)\\ \Rightarrow \frac{dx(t)}{dt} &= A\lambda e^{\lambda t} && (2.131)\\ \text{and} \quad \frac{d^2x(t)}{dt^2} &= A\lambda^2 e^{\lambda t}. && (2.132) \end{aligned}$$

Then can substitute into Eq (2.129):

$$\begin{aligned} MA\lambda^2\exp(\lambda t) + \gamma A\lambda\exp(\lambda t) + \kappa A\exp(\lambda t) &= 0 && (2.133)\\ M\lambda^2 + \gamma\lambda + \kappa &= 0, && (2.134) \end{aligned}$$

where in the last step we divide through by $A\exp(\lambda t)$ since this can't be zero unless we are in the uninteresting case $A = 0$.

What we have shown is that there are solutions of the form $x \propto \exp(\lambda t)$ provided that λ obeys a quadratic equation,

$$M\lambda^2 + \gamma\lambda + \kappa = 0. \tag{2.135}$$

It's convenient to divide through by the mass M, which gives us

$$\lambda^2 + \left(\frac{\gamma}{M}\right)\lambda + \left(\frac{\kappa}{M}\right) = 0. \tag{2.136}$$

This is a quadratic equation, which means that λ can take on two values, which we will call $\lambda_\pm$,

$$\lambda_\pm = \frac{1}{2}\left[-\frac{\gamma}{M} \pm \sqrt{\left(\frac{\gamma}{M}\right)^2 - 4\left(\frac{\kappa}{M}\right)}\right]. \tag{2.137}$$

---

[2] Let's assume that things move slowly enough to make this approximation. You'll look at the case of $F_{\text{drag}} \propto v^2$ in one of the problems.

We will see that these roots of the quadratic are all we need to construct the trajectory $x(t)$.

Before calculating any further it is useful to recall that we have already solved two limits of this problem. When $\gamma = 0$ it is just the harmonic oscillator without damping. Then we see that

$$\begin{aligned} \lambda_\pm(\gamma = 0) &= \frac{1}{2}\left[\pm\sqrt{-4\left(\frac{\kappa}{M}\right)}\right] && (2.138)\\ &= \frac{1}{2}\left[\pm i2\sqrt{\frac{\kappa}{M}}\right] && (2.139)\\ &= \pm i\omega, && (2.140) \end{aligned}$$

where as before we write $\omega = \sqrt{\kappa/M}$. So we recover what we had in the absence of damping, as we should.

Actually we have also solved already another limit, which is $\kappa = 0$, because this is just a particle subject to damping with no other forces. We know that in this case the velocity decays exponentially, $v(t) = v(0)\exp(-\gamma t/M)$, so we should recover $\lambda = -\gamma/M$. But why are there two values of λ? Let's calculate:

$$\begin{aligned} \lambda_\pm(\kappa = 0) &= \frac{1}{2}\left[-\frac{\gamma}{M} \pm \sqrt{\left(\frac{\gamma}{M}\right)^2}\right] && (2.141)\\ &= \frac{1}{2}\left[-\frac{\gamma}{M} \pm \frac{\gamma}{M}\right]. && (2.142) \end{aligned}$$

Thus we see that

$$\lambda_-(\kappa = 0) = \frac{1}{2}\left[-\frac{\gamma}{M} - \frac{\gamma}{M}\right] = -\frac{\gamma}{M}, \qquad (2.143)$$

which is what we expected. On the other hand,

$$\lambda_+(\kappa = 0) = \frac{1}{2}\left[-\frac{\gamma}{M} + \frac{\gamma}{M}\right] = 0. \qquad (2.144)$$

What does this mean? If say that $x(t) \propto e^{\lambda t}$, and $\lambda = 0$, then we are really saying that $x(t) \propto 1$ is a solution—$x(t)$ is constant. This is right, because in the absence of the spring there is nothing to say that the particle should come to rest at $x = 0$; indeed, no particular position is special, and where you stop just depends on where you start. Thus, the solution has a piece that corresponds to adding a constant to the position.

You should see that something interesting has happened: In one limit ($\gamma \to 0$) we have imaginary values of λ and we know that this describes sinusoidal oscillations. In the other limit ($\kappa \to 0$) we have purely real values of λ, and this describes exponential decays, plus constants. Obviously it's interesting to ask how we pass from one limit to the other ... .

One of the important ideas here is that looking at λ itself tells us a great deal about the nature of the dynamics that we will see in the function $x(t)$, even before we finish solving the whole problem. We already know that when λ is imaginary, we will see a sine or cosine oscillation. On the other hand, if λ is a real number and negative, then we will see an exponential decay, as in the case of a mass moving through a viscous fluid. Finally, when λ is real and positive, we see exponential growth, as in the case of a bacterial population (cf Section 1.5). In the present case of the damped harmonic oscillator, we will see cases where λ is real and where it is complex, and we will have to understand what this combination of real and imaginary parts implies about $x(t)$.

Before going any further, let's understand how to use these roots in constructing the full solution $x(t)$. The general principle again is to make a solution by linear combination,

$$x(t) = Ae^{\lambda_+ t} + Be^{\lambda_- t}. \tag{2.145}$$

Then we have to match the initial conditions:

$$\begin{aligned}
x(0) &= A + B, && (2.146)\\
v(0) &\equiv \left.\frac{dx(t)}{dt}\right|_{t=0} && (2.147)\\
&= \left.\left[A\lambda_+ e^{\lambda_+ t} + B\lambda_- e^{\lambda_- t}\right]\right|_{t=0} && (2.148)\\
&= A\lambda_+ + B\lambda_-. && (2.149)
\end{aligned}$$

After a little algebra you can solve these equations to find

$$\begin{aligned}
A &= \frac{\lambda_- x(0) - v(0)}{\lambda_- - \lambda_+} && (2.150)\\
B &= \frac{-\lambda_+ x(0) + v(0)}{\lambda_- - \lambda_+}. && (2.151)
\end{aligned}$$

Problem 37: Derive Eq's (2.150) and (2.151).

Thus the general solution to our problem is

$$x(t) = \frac{[\lambda_- x(0) - v(0)]\exp(\lambda_+ t) + [-\lambda_+ x(0) + v(0)]\exp(\lambda_- t)}{\lambda_- - \lambda_+}. \quad (2.152)$$

Admittedly this is a somewhat complicated looking expression. Let's focus on the case where $v(0) = 0$, so that things get simpler:

$$\begin{aligned} x(t) &= \frac{[\lambda_- x(0)]\exp(\lambda_+ t) + [-\lambda_+ x(0)]\exp(\lambda_- t)}{\lambda_- - \lambda_+} && (2.153) \\ &= x(0)\frac{\lambda_- \exp(\lambda_+ t) - \lambda_+ \exp(\lambda_- t)}{\lambda_- - \lambda_+}. && (2.154) \end{aligned}$$

Notice that it doesn't matter if we exchange λ_+ and λ_-, which makes sense since our choice of the signs $\pm$ in the roots of a quadratic equation is just a convention. Checking for this sort of invariance under different choices of convention is a good way to be sure you haven't made any mistakes!

When we construct $x(t)$, three rather different things can happen, depending on the term under the square root in Eq. (2.137). To see this it is useful to define $\omega_0 = \sqrt{\kappa/M}$ as the "natural frequency" of the oscillator, that is the frequency at which we'd see oscillations if there were no damping. Then

$$\lambda_\pm = \frac{1}{2}\left[-\frac{\gamma}{M} \pm \sqrt{\left(\frac{\gamma}{M}\right)^2 - 4\omega_0^2}\right]. \quad (2.155)$$

Problem 38: Go back to the differential equation that we started with,

$$M\frac{d^2x}{dt^2} + \gamma\frac{dx}{dt} + \kappa x = 0, \quad (2.156)$$

and gives the units for all the parameters M, γ and κ. Then show that what the natural frequency ω_0 really does have the units of frequency or 1/time. What are the units of $\Gamma = \gamma/2M$? Explain why your answer makes sense given the formula for $\lambda_\pm$.

The key point is to look at the square root in the formula for $\lambda_\pm$, Eq (2.155). If $\gamma/M > 2\omega_0$, then the term under the square root is positive, so that its square root is a real number, and hence $\lambda_\pm$ itself is real. Presumably this describes exponential decays—the damping or viscous drag is so large that it destroys the oscillation completely. On the other hand, if $\gamma/M < 2\omega_0$, then the term under the square root is negative and its square root is imaginary. So now $\lambda_\pm$ will be complex numbers. Clearly this is different, and the two cases are called *overdamped* ($\gamma/M > 2\omega_0$) and *underdamped* ($\gamma/M < 2\omega_0$), respectively.

Underdamping. This is the case where the combination under the square root is negative, that is

$$\frac{\gamma}{2M} < \omega_0. \tag{2.157}$$

In this case, $\lambda_\pm$ has an imaginary part,

$$\begin{aligned} \lambda_\pm &= -\frac{\gamma}{2M} \pm i\omega && (2.158) \\ \omega &= \sqrt{\omega_0^2 - \left(\frac{\gamma}{2M}\right)^2}. && (2.159) \end{aligned}$$

This means that the time dependence of x is given by

$$\begin{aligned} x(t) &= A\exp(\lambda_+ t) + B\exp(\lambda_- t) && (2.160) \\ &= A\exp\left(-\frac{\gamma}{2M}t + i\omega t\right) + B\exp\left(-\frac{\gamma}{2M}t - i\omega t\right) && (2.161) \end{aligned}$$

Notice that for x to be real A and B must once again be complex conjugates, so that if $A = |A|\exp(i\phi_A)$ as before, we can write

$$\begin{aligned} x(t) &= A\exp\left(-\frac{\gamma}{2M}t + i\omega t\right) + \left[A\exp\left(-\frac{\gamma}{2M}t + i\omega t\right)\right]^* && (2.162) \\ &= |A|\exp\left(+i\phi_A - \frac{\gamma}{2M}t + i\omega t\right) \\ &\qquad + \left[|A|\exp\left(+i\phi_A - \frac{\gamma}{2M}t + i\omega t\right)\right]^* && (2.163) \\ &= 2\mathrm{Re}\left[|A|\exp\left(+i\phi_A - \frac{\gamma}{2M}t + i\omega t\right)\right] && (2.164) \\ &= 2|A|\exp\left(-\frac{\gamma}{2M}t\right)\cos(\omega t + \phi_A) && (2.165) \end{aligned}$$

We see that the introduction of damping causes oscillations to occur at a lower frequency, since $\omega < \omega_0$, and causes these oscillations to decay according to the exponential 'envelope' outside the cosine. See Fig. 2.6.

Overdamping. This is when

$$\frac{\gamma}{2M} > \omega_0, \tag{2.166}$$

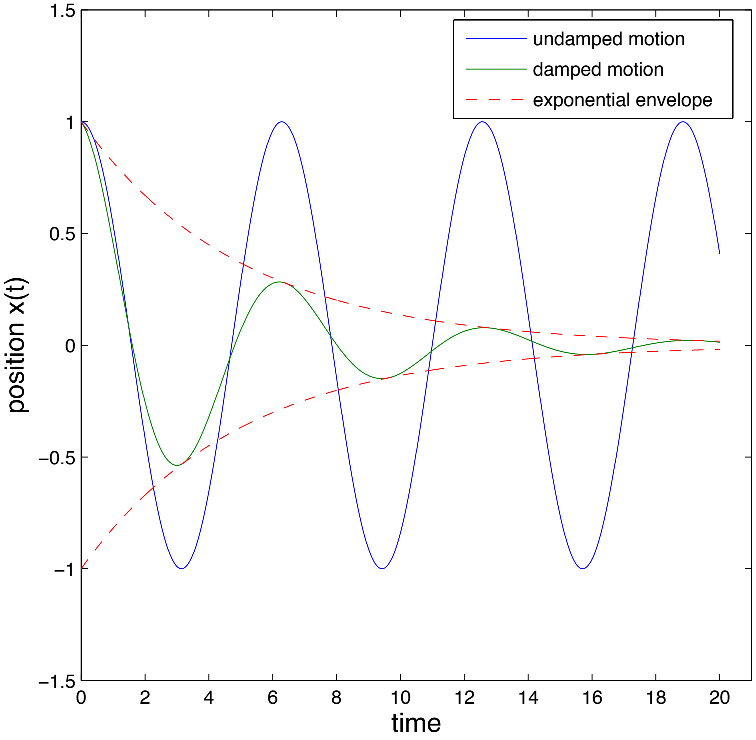


Figure 2.6: Comparing the motion of a damped oscillator, following the predictions from Eq (2.165), with that of an undamped oscillator (same equation but with $\gamma = 0$). We choose units such that $\omega_0 = 1$, and for the damped oscillator we take $\gamma/2M = 0.2$; in both cases the initial phase $\phi_A = 0$.

and now the term inside the square root in Eq (2.155) is positive. This means that both λ_+ and λ_- are real, and in fact both are negative. Thus we can write $\lambda_+ = -|\lambda_+$ and $\lambda_- = -|\lambda_-$, so that

$$x(t) = A\exp(-|\lambda_+|t) + B\exp(-|\lambda_-|t). \tag{2.167}$$

Thus the displacement consists just of decaying exponentials, and hence there is **no** oscillation.

To understand what happens it is convenient to go into the *strongly* overdamped limit, where $\gamma/(2M) \gg \omega_0$. Then we can do some algebra to work out the values of $\lambda_\pm$. The easy case is λ_-:

$$\begin{aligned}
\lambda_-(\gamma/(2M) \gg \omega_0) &= \frac{1}{2}\left[-\frac{\gamma}{M} - \sqrt{\left(\frac{\gamma}{M}\right)^2 - 4\omega_0^2}\right] \\
&\approx \frac{1}{2}\left[-\frac{\gamma}{M} - \sqrt{\left(\frac{\gamma}{M}\right)^2}\right] \qquad (2.168) \\
&= -\frac{\gamma}{M}. \qquad (2.169)
\end{aligned}$$

Notice that in this case we implement that approximation $\gamma/(2M) \gg \omega_0$ just by neglecting ω_0^2 relative to $(\gamma/2M)^2$ under the square root. To estimate λ_+ in this limit we have to be a bit more careful, and make use of a Taylor series expansion for the square root.

Problem 39: In general, for small a,

$$\sqrt{1+a} = 1 + \frac{1}{2}a - \frac{1}{8}a^2 + \cdots . \qquad (2.170)$$

Derive this expression using the Taylor expansion. When we say that a is "small," you might wonder how small it needs to be. Plot the exact function $\sqrt{1+a}$ vs a, say in the range $-1 < a < 1$, and compare with the approximate expression. When can you get away with just saying $\sqrt{1+a} \approx 1 + a/2$? How much does the second term ($\sim a^2$) help? Can you go a third term and do better?

To carry out the approximation, it's useful to rearrange things a bit at the beginning:

$$\begin{aligned}
\lambda_- &= \frac{1}{2}\left[-\frac{\gamma}{M}+\sqrt{\left(\frac{\gamma}{M}\right)^2-4\omega_0^2}\right] && (2.171)\\
&= \frac{1}{2}\left[-\frac{\gamma}{M}+\sqrt{\left(\frac{\gamma}{M}\right)^2\left(1-4\left(\frac{\omega_0}{\gamma/M}\right)^2\right)}\right] && (2.172)\\
&= \frac{1}{2}\left[-\frac{\gamma}{M}+\frac{\gamma}{M}\sqrt{1-4\left(\frac{\omega_0}{\gamma/M}\right)^2}\right] && (2.173)\\
&= \frac{\gamma}{2M}\left[-1+\sqrt{1-4\left(\frac{\omega_0}{\gamma/M}\right)^2}\right] && (2.174)\\
&\approx \frac{\gamma}{2M}\left[-1+1-\frac{1}{2}4\left(\frac{\omega_0}{\gamma/M}\right)^2+\cdots\right] && (2.175)\\
&= -\frac{\gamma}{2M}\frac{1}{2}4\left(\frac{\omega_0}{\gamma/M}\right)^2=\frac{M\omega_0^2}{\gamma} && (2.176)\\
&= \frac{\kappa}{\gamma}. && (2.177)
\end{aligned}$$

The key steps were to use the Taylor expansion of the square root,

$$\sqrt{1-x}\approx 1-\frac{1}{2}x+\cdots\,, \qquad (2.178)$$

and to notice that since the natural frequency is given by $\omega_0^2=\kappa/M$, we have $M\omega_0^2=\kappa$. To summarize, in the extreme overdamped limit, we have

$$x(t)=A\exp\left(-\frac{\gamma}{M}t\right)+B\exp\left(-\frac{\kappa}{\gamma}t\right). \qquad (2.179)$$

Notice that both are exponential decays, one gets faster at large γ and one gets slower at large γ. Intuitively, the fast decay is the loss of inertia (forgetting the initial velocity) and the slow decay is the relaxaton of the spring back to its equilibrium position. Roughly speaking, γ/M is the rate at which the initial velocity is forgotten, while κ/γ describes the slow relaxation of the position back to equilibrium at $x=0$.

Problem 40: If the interpretation we have just given for the behavior of $\lambda_\pm$ in the overdamped limit is correct, then the decay of the velocity gets faster as γ gets larger, while the decay of the position gets slower. Explain, intuitively, why this makes sense.

To be sure that this interpretation is correct, consider the case where the initial velocity is zero, which case we should see relatively little contribution from the term $\sim \exp(-\gamma t/M)$. To satisfy the initial conditions we must have

$$\begin{aligned}
0 &= \left.\frac{dx(t)}{dt}\right|_{t=0} && (2.180)\\
&= \frac{d}{dt}\left[A\exp\left(-\frac{\gamma}{M}t\right)+B\exp\left(-\frac{\kappa}{\gamma}t\right)\right]\Bigg|_{t=0} && (2.181)\\
&= \left[A\left(-\frac{\gamma}{M}\right)\exp\left(-\frac{\gamma}{M}t\right)+B\left(-\frac{\kappa}{\gamma}\right)\exp\left(-\frac{\kappa}{\gamma}t\right)\right]\Bigg|_{t=0} && (2.182)\\
&= -A\frac{\gamma}{M}-B\frac{\kappa}{\gamma} && (2.183)\\
\Rightarrow A\frac{\gamma}{M} &= -B\frac{\kappa}{\gamma} && (2.184)\\
A &= -B\frac{M\kappa}{\gamma^2} = -B\frac{M\cdot M\omega_0^2}{\gamma^2} = -B\left(\frac{M\omega_0}{\gamma}\right)^2. && (2.185)
\end{aligned}$$

Thus we see that in the strongly overdamped limit, where $\gamma \gg M\omega_0$, we have $A \ll B$ if the initial velocity is zero, as promised.

Problem 41: Many proteins consist of separate "domains," often with flexible connections between the domains. Imagine a protein that is sitting still, with one extra domain that can move. Assume that this mobile domain is roughly spherical with a radius of $r \sim 1\,\text{nm}$, and that it has a molecular weight $m \sim 30,000\,\text{a.m.u.}$.[3] The small piece of the molecule which connects this domain to the rest of the protein acts like a spring with stiffness $\kappa \sim 1\,\text{N/m}$.

(a.) If there were no drag, what differential equation would describe the motion of the domain? Would the domains oscillate? At what frequency?

(b.) Estimate the drag coefficient for motion of the domain through water. You should use Stokes' formula, which you explored in the lab.

---

[3] Reminder: one mole of atomic mass units (a.m.u.) has a total mass of one gram.

(c.) Write out the differential equation that describes motion in the presence of damping. Given the parameters above, is the resulting motion of the domain underdamped or overdamped?

(d.) If the spring that attaches the mobile domain to the rest of the protein is stretched and released with zero velocity, estimate how much time it takes before this displacement decays to half its initial value.

Problem 42: In your ear, as in the ears of other animals, the "hair cells" which are sensitive to sound have a bundle of small finger–like structures protruding from their surface. These hairs, or stereocilia, bend in response to motion of the surrounding fluid. Directly pushing on the hairs one measures a stiffness of $\kappa \sim 10^{-3}\,\mathrm{N/m}$. In this problem you'll examine the possibility that the stereocilia form a mass–spring system that resonates in the $\omega_0 \sim 2\pi \times 10^3\,\mathrm{Hz}$ frequency range that corresponds to the most sensitive range of human hearing.

(a.) What mass would the stereocilia have to have in order that their natural frequency would come out to be $\omega_0 \sim 2\pi \times 10^3\,\mathrm{Hz}$?

(b.) The entire bundle of stereocilia in human hair cells ranges from 1 to $5\,\mu\mathrm{m}$ in height, and the cross–sectional area of the bundle typically is less than $1\,\mu\mathrm{m}^2$. Is it plausible that this bundle has the mass that you derived in [a]? You'll need to make some assumptions about the density of the hairs, and you should state your assumptions clearly.

(c.) Independent of your answer to [b], it still is possible that the stiffness of the stereocilia is the spring in mass–spring resonance, perhaps with the mass provided by some other nearby structure. But when the stereocilia move through the fluid, this will generate a damping or drag coefficient γ. How small would γ have to be in order that this system exhibit a real resonance?

(d.) The geometry of the stereocilia is complicated, so actually calculating γ is difficult. You know that for spherical objects $\gamma = 6\pi\eta R$, with R the radius and η the viscosity of the surrounding fluid (water, in this case). You also experimented with objects of different shape and learned something about how damping coefficients depend on size and shape. Using what you know, decide whether γ for the stereocilia can be small enough to satisfy the conditions for underdamping that you derived in [c].

Problem 43: For the damped harmonic oscillator,

$$m\frac{d^2x}{dt^2} + \gamma\frac{dx}{dt} + \kappa x = 0, \tag{2.186}$$

we found that the solution can be written as $x(t) = Ae^{\lambda_+ t} + Be^{\lambda_- t}$, where $\lambda_\pm$ are the roots of a quadratic equation, $m\lambda^2 + \gamma\lambda + \kappa = 0$.

(a.) Find the constants A and B in the case where the initial conditions are $x(t) = 1$ and $(dx/dt)|_{t=0} = 0$. Write the function $x(t)$ only in terms of $\lambda_\pm$.

(b.)To be sure you understand what underdamping and overdamping really mean, we'd like you to plot the function $x(t)$ in different cases. To make things clear, choose units of time so that $\kappa/m = 1$. Then if $\gamma = 0$ you should just have $x(t) = \cos(t)$. Now consider values of $\gamma/2m = 0.1, 0.9, 1.1, 10$. In each case, use MATLAB to plot $x(t)$ over some interesting range of times; part of the problem here is for you to decide what is interesting.

(c.) Write a brief description of your results in [b]. Can you show the slowing of oscillations in the presence of a small amount of drag? The exponential envelope for the decay? The disappearance of oscillations in the overdamped regme?

(d.) Use your mathematical expression for $x(t)$ to explore what happens right at the transition between overdamped and underdamped behavior ("crtitical damping"), where

$\lambda_+ = \lambda_-$. Hint: Recall l'Hopital's rule, which states that if two functions $f(y)$ and $g(y)$ are both zero at $y = y_0$, then

$$\lim_{y\to y_0} \frac{f(y)}{g(y)} = \frac{f'(y_0)}{g'(y_0},\tag{2.187}$$

where $f'(y_0)$ is another way of writing $(df/dy)|_{y=y_0}$. Hopefully you will discover that, in addition to sines, cosines and exponentials, this gives yet another functional form. It seems remarkable that by varying parameters in one equation we can get such different predictions. Maybe even more remarkable is that we can capture this wide range of behaviors by using the complex exponentials, although we do have to use them carefully.

Problem 44: So far we have discussed damping of the harmonic oscillator in the case where the damping is linear, $F_{\rm drag} = -\gamma v$. What happens if $F_{\rm drag} = -cv^2$? In an oscillator, the velocity changes sign during each period of oscillation, so we should be careful and write $F_{\rm drag} = -c|v|v$ so that the drag force always opposes the motion. Then the relevant differential equation is

$$M\frac{d^2x(t)}{dt^2} + c\left|\frac{dx(t)}{dt}\right|\frac{dx(t)}{dt} + \kappa x(t) = 0,\tag{2.188}$$

where as usual M is the mass and κ is the stiffness of the spring to which the mass is attached. Consider an experiment in which we stretch the spring to an initial displacement $x(0) = x_0$ and release it with zero velocity.

(a.) This problem seems to have lots of parameters: M, c, κ and x_0. It's very useful to simplify the problem by changing units, so you can see that there really aren't so many parameters. Consider measuring position in units of the initial displacement, $X = x/x_0$ and measuring time in units related to the period of the oscillations, $T = \omega t$, where as usual $\omega = \sqrt{\kappa/M}$. Show that Eq (2.188) is equivalent to

$$\frac{d^2X}{dT^2} + B\left|\frac{dX}{dT}\right|\frac{dX}{dT} + X = 0,\tag{2.189}$$

where B in a dimensionless combination of parameters. What is the formula for B is relation to all the original parameters?

(b.) Write a simple program in MATLAB to solve Eq (2.189). Clearly you will need to choose time steps $\Delta T \ll 1$, but you don't know in advance what to choose so leave this as a parameter.

(c.) Small values of B should generate relatively small amounts of damping. Try $B = 0.1$, and run your program for a time long enough to see 20 oscillations; a reasonable value for the time step is $\Delta T = 0.01$. Can you see the effects of the damping? Does it look different from the case of linear damping?

(d.) Do some numerical experiments to see if the choice $\Delta T = 0.01$ really gives a reliable solution.

(e.) With linear damping, there is a critical value that destroys the oscillation and leads to "overdamping." Try increasing the value of B and running your program to see if there is a similar transition in the case of nonlinear damping.

(f.) Is $\Delta T = 0.01$ still sufficiently small as you explore larger values of B?

2.4 Linearization and stability

The harmonic oscillator is an interesting problem, but we don't teach you about it because we expect you to encounter lots of masses and springs in your scientific career. Rather, it is an example of how one can analyze a system to reveal its stability and oscillations. To place this in a more general context, realize that our standard problem

$$m\frac{d^2x}{dt^2} + \gamma\frac{dx}{dt} + \kappa x = 0 \tag{2.190}$$

is a linear differential equation with constant coefficients. "Linear" because the variable x appears only raised to the first power (that is, there are no terms like x^2 or x^3), and "constant coefficients" because there is no explicit dependence on time. We have learned that equations like this can be solved by looking for solutions of the form $x(t) = Ae^{\lambda t}$, and that such solutions can be found provided that λ takes on some very specific values. If the allowed values of λ have imaginary parts, then this signals an oscillation. If the real part of λ is negative, then any initial displacement will decay with time, while if the real part of λ were positive this would mean that initial displacements grow—in fact blow up—with time (although we haven't seen an example of this yet). In this lecture we'd like to show you how these same ideas can be used in very different contexts.

Consider the all too familiar interaction between a loudspeaker and a microphone, as sketched in Fig 2.7. A modern electrostatic loudspeaker is essentially a stiff plate, and when we apply a voltage $V(t)$ this generates a force on the plate. So the equation describing the displacement $x(t)$ of the plate is pretty simple:

$$\kappa x(t) = aV(t), \tag{2.191}$$

where the constant a is a property of the particular loudspeaker we are looking at.[4] When the loudspeaker moves, it generates a sound pressure $p(t)$ where we are standing. But because sound propagates through the air at finite speed, the sound pressure that the microphone detects at time t must be related to the motion of loudspeaker at some time $t - \tau$ in the past, where τ is the time for propagation of the sound waves. Again this is a

---

[4] Clearly this can't be exactly true: If we change the voltage quickly enough, the plate can't possibly follow instantaneously. But it's a good approximation over some range of conditions that we care about in practice, and in fact loudspeakers are designed in part to make this a approximation work as well as possible.

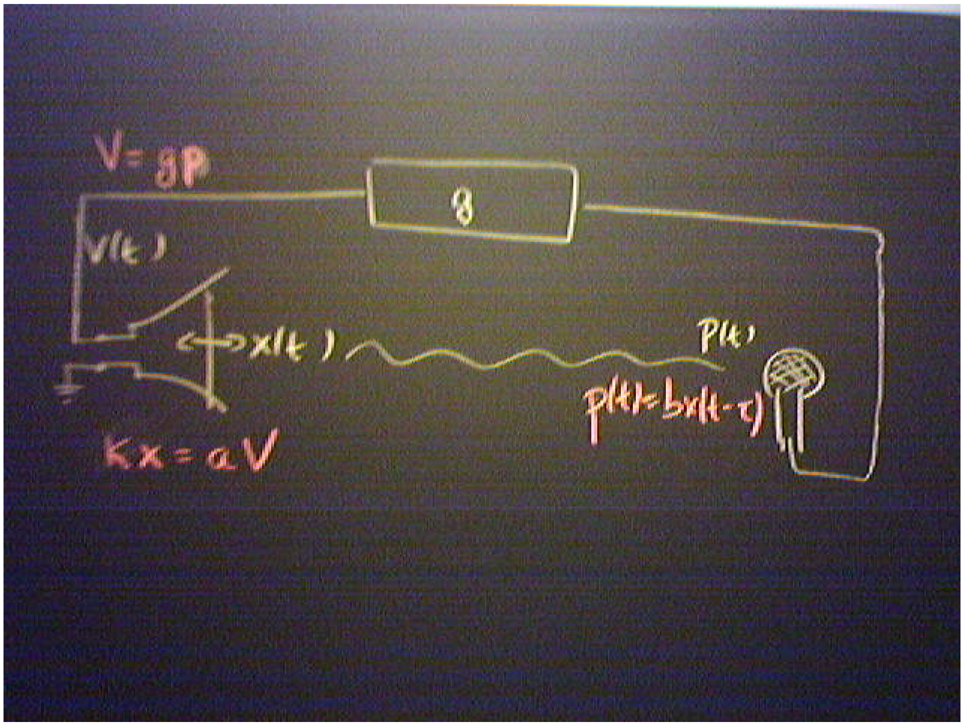


Figure 2.7: A loudspeaker generates sound, and a microphone picks up these signals. Inevitably, there is some feedback. In the text we analyze this to explain the howling instabilities that we all have experienced.

simplification, since in the real world there are many paths from loudspeaker to microphone (echoing off the walls of the room, for example), each of which has its own time delay; here we're going to approximate that there is just one path with one delay. Thus we have

$$p(t) = bx(t - \tau), \tag{2.192}$$

where b is a constant that measures the efficiency of the loudspeaker.

The whole point of the the microphone, of course, is that sound pressure gets converted into an electrical voltage that we can use to drive the loudspeaker. There is some factor g that expresses the "gain" in this transformation; if we have an amplifier in the system then turning the knob on the amplifier adjusts this gain:

$$V(t) = gp(t). \tag{2.193}$$

Putting all of these thing together we have

$$\begin{aligned} \kappa x(t) &= aV(t) \\ &= agp(t) \qquad (2.194) \\ &= agbx(t-\tau) \qquad (2.195) \\ x(t) &= \frac{agb}{\kappa}x(t-\tau). \qquad (2.196) \end{aligned}$$

It's useful to call the combination of parameters $agb/\kappa = G$, so the dynamics of our system is determined simply by

$$x(t) = Gx(t-\tau). \qquad (2.197)$$

It is interesting that Eq (2.197) looks nothing like the differential equations we have been solving. In fact, there are no derivatives, just a delay. Still, the equation is linear, so we might try our usual trick of looking for solutions in the form $x(t) = Ae^{\lambda t}$. Substituting, we find:

$$\begin{aligned} x(t) &= Gx(t-\tau) \\ Ae^{\lambda t} &= GAe^{\lambda(t-\tau)} \qquad (2.198) \\ &= GAe^{-\lambda\tau}e^{\lambda t}. \qquad (2.199) \end{aligned}$$

As usual, we can divide through by A and by $e^{\lambda t}$, to obtain

$$1 = Ge^{-\lambda\tau}, \qquad (2.200)$$

or equivalently

$$e^{\lambda\tau} = G. \qquad (2.201)$$

This looks easy to solve: take the (natural) log of both sides, then divide through by τ:

$$\begin{aligned} e^{\lambda\tau} &= G \\ \lambda\tau &= \ln G \qquad (2.202) \\ \lambda &= \frac{\ln G}{\tau}. \qquad (2.203) \end{aligned}$$

We see that if $G < 1$, then λ will be negative, but if $G > 1$ then λ will positive. Since our solutions are of the form $x(t) \sim e^{\lambda t}$, positive λ means that the displacement of the loudspeaker will blow up with time. This certainly starts to seem like an explanation of what happens in real life: if we have too large a gain in our amplifier (g and hence G is too big), then the "feedback" from microphone to amplifier can lead to an instability in which the system starts to make its own sounds. The sound pressure can rise from the point where we barely hear it to the point where it is painful, which corresponds to p or x growing by a factor of 10^6.

Actually we don't quite have a theory of the blow up in our audio system. So far, $x(t)$ is growing exponentially, but it's not oscillating. We know that the real instabilities of audio systems occur with the sound pressure oscillating at some frequency, since we hear (admittedly badly tuned) 'notes' or whistles. Are these somehow hiding in our equations?

We are trying to solve the equation $\exp(\lambda\tau) = G$. We have found one solution, but is this the unique solution? Recall that

$$\exp(2\pi i) = 1, \tag{2.204}$$

and also that

$$[\exp(2\pi i)]^2 = \exp(4\pi i) = 1, \tag{2.205}$$

and so on, so that

$$\exp(2n\pi i) = 1, \tag{2.206}$$

for any integer $n = \pm 1, \pm 2, \pm 3, \cdots$. This means that once we open our minds to complex numbers, taking logarithms is no longer so easy. For example, we can write that

$$e^{\ln 3} = 3. \tag{2.207}$$

But it's also true that

$$e^{\ln 3} e^{2\pi i} = e^{\ln 3 + 2\pi i} = 3. \tag{2.208}$$

So when take the natural log of 3 we might mean what we always meant by the number $\ln 3$, but we might also mean $\ln 3 + 2\pi i$, and it's worse because we could mean $\ln 3 \pm 2\pi i$, $\ln 3 \pm 4\pi i$, and so on. All this craziness means that our simple equation $\exp(\lambda\tau) = G$ actually has many solutions:

$$\begin{aligned} \lambda\tau &= \ln G \pm 2n\pi i && (2.209) \\ \lambda &= \frac{\ln G}{\tau} \pm i\frac{2n\pi}{\tau}, && (2.210) \end{aligned}$$

where $n = 0, 1, 2, \cdots$. Now we see that λ can have imaginary parts, at frequencies which are integer multiples of $\omega = 2\pi/\tau$.

So, what we have seen is that our trick of looking for solutions in the form $x \sim e^{\lambda t}$ allows to understand what happens in the microphone–loudspeaker system. There are oscillations with a frequency such that the period matches the delay, which makes sense because this is the condition that the signal from the microphone reinforces the motion of the loudspeaker. In fact there isn't a single frequency, but a whole set of "harmonics" at integer multiples of a "fundamental" frequency, just like when we play a note on a musical instrument—this idea of harmonics will reappear when we discuss waves on a string, a few lectures from now. If the gain of the amplifier in the system is small, then these oscillations die away, but if the gain becomes too large then there is an instability and the amplitude of the oscillations will grow exponentially. Presumably this is stopped by the fact that amplifier can't put out infinite power.

Problem 45: The time τ which appears in our analysis of the loudspeaker and microphone is the time for sound to propagate from one element to the other. Given that the speed of sound is 330 m/s in air, what are typical values of τ in a classroom? The difference between a barely audible sound and one that is painful is a factor of $\sim 10^6$ in p; if we set the amplifier so that the gain $G = 2$, how long should it take for the signal to grow by this amount? Does this make sense in terms of your experience?

Problem 46: One can think of the mechanics of muscles as having two components—a passive part that is mostly stiffness and drag, and an active part in which the muscle generates extra force when you pull on it. If we call this active force $F_{\text{active}}(t)$, then the length of the muscle should obey the differential equation

$$\gamma \frac{dL(t)}{dt} + \kappa L(t) = F_{\text{active}}(t), \tag{2.211}$$

where as usual γ describes the drag and κ the stiffness. Consider a simple model for the dynamics of $F_{\text{active}}(t)$: The active force acts like a stiffness, but it takes a little while to develop in response to the changes in muscle length. An equation that can describe this is

$$\tau \frac{dF_{\text{active}}(t)}{dt} + F_{\text{active}}(t) = -\kappa' L(t), \tag{2.212}$$

where τ is (roughly) the time it takes for the active force to develop and κ' is the "active stiffness." Look for a solution of the form $L(t) = L_0 \exp(\lambda t)$ and $F_{\text{active}}(t) = F_0 \exp(\lambda t)$.

(a.) Show that a solution of this form does work provided that L_0, F_0 and λ obey some conditions. Write these conditions as two equations for these three variables.

(b.) Show that the two equations you found in [a] are equivalent to a single quadratic equation for λ, as in the case of the harmonic oscillator. Hint: First use one of the equations to solve for F_0, then substitute into the second equation. You should find that L_0 drops out, leaving just one equation for λ.

(c.) In general, what is the condition on λ that corresponds to underdamped oscillations?

(d.) For this particular problem, what is the condition that all the parameters have to obey in order to generate underdamped oscillations? If the "active stiffness" κ' is big enough, will this generate oscillations?

(e.) Does anything special happen when the time scale for the active force τ matches the time scale for relaxation of the passive dynamics, $\tau_0 = \gamma/\kappa$?

Problem 47: There is a process that synthesizes molecule A at a constant rate s (as in "zeroth order" kinetics). Once synthesized, these molecules decay into B with a first order rate constant k_{AB}, and B decays into C with another first order rate constant k_{BC}:

$$\overset{s}{\rightarrow} A \overset{k_{AB}}{\rightarrow} B \overset{k_{BC}}{\rightarrow} C. \tag{2.213}$$

The B molecules also have the unusual feature that they act as a catalyst, causing A to convert directly into C through a second order reaction with rate constant k_2:

$$A + B \overset{k_2}{\rightarrow} C + B. \tag{2.214}$$

(a.) What are the units of all the parameters in the problem, s, k_{AB}, k_{BC} and k_2?

(b.) Write out the differential equations that describe the concentrations of A and B. Start by assuming $k_2 = 0$, so that only the reactions in (1) are occurring. How are the equations changed by including the catalytic reaction in (2)?

(c.) Find the steady state concentrations, $[A] = \bar{A}$ and $[B] = \bar{B}$, that will stay unchanged over time. Again, start with the easier case in which $k_2 = 0$ and then see how things change when the catalytic reaction is significant.

(d.) Assume that concentrations of A and B are close to their steady state values, and find the linear differential equations that describe the final approach to the steady state. Hint: think about the approach to terminal velocity in mechanics. Note: You can keep these equations in terms of $\bar{A}$ and $\bar{B}$; there is no need to substitute from [c].

(e.) Show that if $k_2 = 0$, then the concentrations of A and B will relax to their steady state values as exponential decays.

(f.) Can the equations in [d] describe oscillations when we include the effects of k_2?

To emphasize the generality of these ideas, let's look at something completely different. Every cell in your body has the same DNA. Sequences along the DNA code for proteins, but what makes different cells (e.g., in your liver and your brain) different from one another is that they *express* different proteins. You recall from your high school biology classes that to make protein, the cell first transcribes the relevant segment of DNA into messenger RNA, and then this is translated into protein. One way that the cell regulates this process is to have other proteins, called transcription factors, bind to the DNA and inhibit or assist the process of transcription. Sweeping lots of things under the rug, one can make a sketch as in Fig 2.8, showing how the rate of protein synthesis for a particular gene depends on the concentration of the transcription factor.

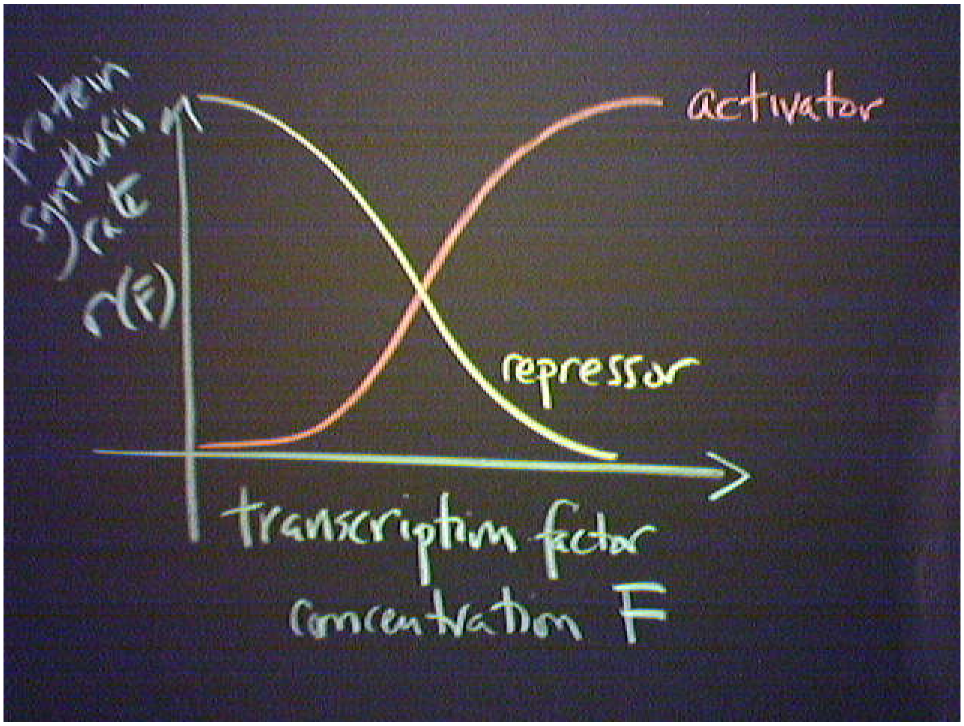


Figure 2.8: Regulation of gene expression. In the simplest picture, proteins are synthesized at a rate $r(F)$ that depends on the concentration F of some transcription factor. The transcription factor can be an activator or a repressor.

If we take the sketch in Fig 2.8 seriously, we can write the rate of protein synthesis as $r(F)$, where F is the concentration of the transcription factor. Once the proteins are made, they also are degraded by a variety of processes, and let's assume that we can lump all these together into some first order rate constant k for degradation. Then the dynamics of protein concentration are given by

$$\frac{dP}{dt} = r(F) - kP. \tag{2.215}$$

Of course, the transcription factor is itself a protein, and so some similar dynamics are being played out at another point along the genome. The real problem of understand the dynamics of transcriptional regulation is to think about these coupled dynamics of different genes. But, to get a feeling for what can happen, let's make a drastic simplification and imagine that the protein we are looking at actually regulates itself. Then "the transcription

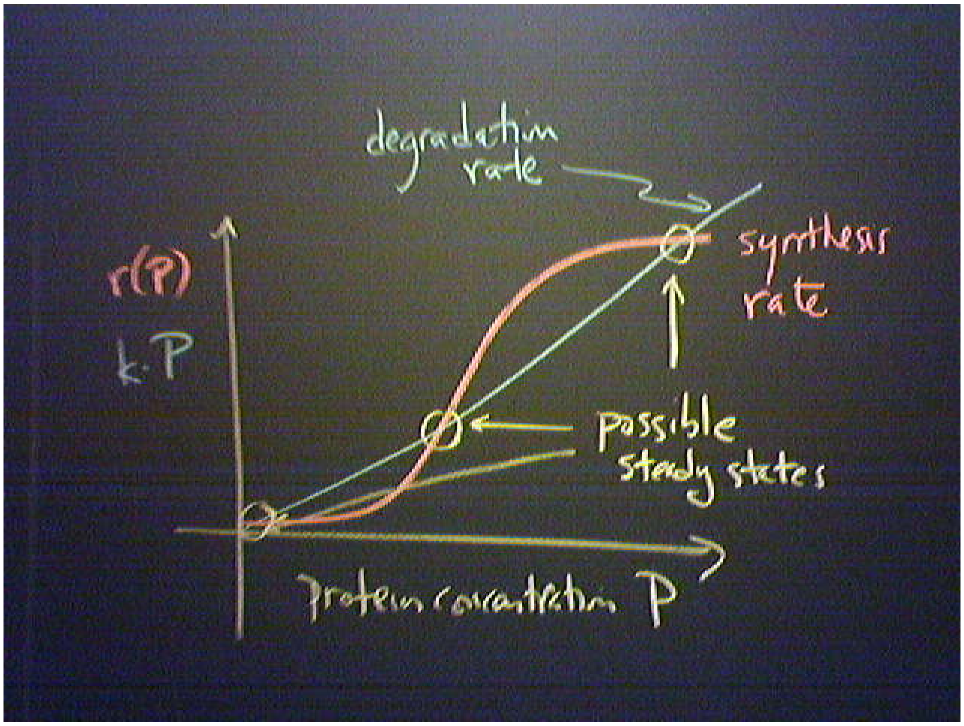


Figure 2.9: Steady states of a gene that activates its own expression. With dynamics as in Eq (2.216), steady states are possible when the rate of protein synthesis $r(P)$ balances the rate of degradation kP. With the parameters chosen here, there are three possible steady states.

factor" really is the protein we have been discussing, and hence $F = P$; the dynamics then are described by

$$\frac{dP}{dt} = r(P) - kP. \tag{2.216}$$

Just to be clear, there is no case in nature that is quite this simple. On the other hand, there are examples that aren't too much more complicated (e.g., two proteins which regulate each other), and with modern methods of molecular biology one can engineer bacteria to implement something like the simple model we are discussing here. So, it's oversimplified, but maybe not ridiculously oversimplified (!).

How, then, do we attack a model like that in Eq (2.216)? We can start by asking if there is any way for the system to come to a steady state. This will happen when $dP/dt = 0$, which is equivalent to $r(P) = kP$. Let's consider the case of an activator. Then graphically our problem is shown in Fig 2.9.

We can plot $r(P)$ vs P, and we can also plot kP vs P (the last plot just being a straight line). Whenever these two plots cross, we have a possible steady state. At least in some range of parameters, it's clear that there are three possible steady states.

Now we know that not all steady states are created equal. If we balance a ball on top of a hill, there is no force and so it will stay there forever—as long as nobody kicks it. On the other hand, if the ball is sitting at the bottom of a valley, even kicking it a little bit doesn't change anything, since after a while it will roll back to the bottom of the valley and come to rest. We say that the bottom of the valley is a stable steady state, the top of the hill is an unstable steady state. Sometimes we call these steady states "fixed points" of the dynamics. So it's natural to ask, of the three fixed points in our problem (Fig 2.9), which ones are stable and which ones are unstable?

To examine the stability of steady states let's do the mathematical version of giving the ball a small kick. Suppose that we have identified a steady state P_0. Imagine that $P = P_0 + \delta P(t)$, where the difference δP is going to be small. We can derive an equation which describes the dynamics of δP by substituting into Eq (2.216):

$$\begin{aligned}
\frac{dP}{dt} &= r(P) - kP \\
\frac{d(P_0 + \delta P)}{dt} &= r(P_0 + \delta P) - k(P_0 + \delta P) && (2.217) \\
\frac{d(P_0)}{dt} + \frac{d(\delta P)}{dt} &\approx r(P_0) + \left.\frac{dr(P)}{dP}\right|_{P=P_0} \cdot \delta P - kP_0 - k\delta P, && (2.218)
\end{aligned}$$

where in the last step we have used a Taylor series expansion to approximate $r(P)$ in the neighborhood of P_0; since δP is small we just stop with the first term.

Now we can simplify things in Eq (2.218) considerably. To begin, P_0 is a number, so taking its derivative with respect to time gives us zero, so that we have

$$\frac{d(\delta P)}{dt} \approx r(P_0) + \left.\frac{dr(P)}{dP}\right|_{P=P_0} \cdot \delta P - kP_0 - k\delta P. \tag{2.219}$$

Next we notice that we can group the terms together on the right hand side:

$$\frac{d(\delta P)}{dt} \approx [r(P_0) - kP_0] + \left[\left.\frac{dr(P)}{dP}\right|_{P=P_0} - k\right] \delta P. \tag{2.220}$$

But P_0 was defined to be a steady state, which means that $r(P_0) = kP_0$, and hence the first term in $[\cdots]$ vanishes. All we have left is

$$\frac{d(\delta P)}{dt} = \left[\left. \frac{dr(P)}{dP} \right|_{P=P_0} - k \right] \delta P, \tag{2.221}$$

and if we remember that δP has to be small, then it's OK to write $=$ instead of $\approx$.

But we have seen Eq (2.221) before, in other forms. This equation is just

$$\frac{d(\delta P)}{dt} = \alpha \delta P, \tag{2.222}$$

where the constant

$$\alpha = \left[\left. \frac{dr(P)}{dP} \right|_{P=P_0} - k \right]. \tag{2.223}$$

We know the solution of Eq (2.222), it's just $\delta P(t) = \delta P(0) \exp(\alpha t)$. So if $\alpha < 0$ the fixed point P_0 is stable, since a small kick away from the steady state will decay away. If on the other hand we have $\alpha > 0$, the fixed point P_0 is unstable, since a small kick away from the steady state will grow, much as with the ball on top of the hill. The conclusion from all of this is that the steady state protein concentration P_0 will be stable if $dr(P)/dP$ is less than k when we evaluate it at $P = P_0$. Looking at Fig 2.9, we can see that the two fixed points at large and small P satisfy this condition; the intermediate fixed point does not. This means that really we have a "bistable" system, in which there are exactly two stable states separated by an unstable point. This is like having two valleys separated by a hill—you can sit stably in either valley, and you'll always fall into one or the other, depending on which side of the mountain top you find yourself.

Problem 48: Let's fill in the details of the calculation above using a more concrete model. Specifically, let's formalize the sketches of the function $r(F)$ in Fig 2.8, by writing equations for $r(F)$ that look like our sketches:

$$\begin{aligned} r_{\rm act}(F) &= r_{\rm max} \frac{F^n}{F^n + F^n_{1/2}}, & (2.224) \\ r_{\rm rep}(F) &= r_{\rm max} \frac{F^n_{1/2}}{F^n + F^n_{1/2}}. & (2.225) \end{aligned}$$

(a.) Plot[5] the functions $r_{\rm act}(F)$ and $r_{\rm rep}(F)$. Explain the significance of the parameters $r_{\rm max}$ and $F_{1/2}$.

(b.) Consider the case of "auto–regulation," in which the protein is its own transcription factor, so that $P = F$. As discussed above, the case of activator can have three steady states where $dP/dt = 0$. Show that for the repressor there is only one steady state. You should be able to make a qualitative, graphical argument, and then use the equations to make things precise.

(c.) Let the steady state that you found in [c] correspond to $P = P_0$. Assume that $P(t) = P_0 + \delta P(t)$ and derive an approximate, linear equation for $\delta P(t)$ assuming that it is small. How small does it nee to be in order for your approximation to be accurate?

(d.) Solve the linear equation from [c]. How does the behavior of the solution depend on the parameters $r_{\rm max}$, n, $F_{1/2}$, and k?

Problem 49: Let's continue the analysis of a self–activating gene. We have written the dynamics of the protein concentration P as

$$\frac{dP}{dt} = r(P) - kP, \tag{2.226}$$

where k is the first order rate constant for degradation of the protein, and $r(P)$ is the rate of protein synthesis, which depends on P because the protein acts as its own activator. To be explicit, we consider the functional form

$$r(P) = r_{\rm max}\frac{P^n}{P^n + F^n_{1/2}}. \tag{2.227}$$

(a.) Consider normalized variables $p = P/F_{1/2}$ and $\tau = kt$. Show that

$$\frac{dp}{d\tau} = a\frac{p^n}{p^n+1} - p, \tag{2.228}$$

and give a formula that relates a to the original parameters in the problem.

(b.) Consider the specific case $n = 3$. Notice that the condition for a steady state can written as the problem of finding the roots of a polynomial:

$$\begin{aligned} 0 &= a\frac{p^n}{p^n+1} - p && (2.229)\\ p &= a\frac{p^n}{p^n+1} && (2.230)\\ p^{n+1} + p &= ap^n && (2.231)\\ p^{n+1} - ap^n + p &= 0. && (2.232) \end{aligned}$$

Find all the steady state values of p, and plot these as a function of the parameter a. You might find the MATLAB function `roots` to be useful here. Be careful about whether the solutions you find are real! Can you verify that there are three steady states, as explained in the notes? What is the condition on a for this to be true? What happens when this condition is violated?

(c.) Write a program that solves Eq (2.228).

---

[5] Since we already have the sketches, "plot" here means to use a computer to get exact values and plot the results. Think about how to choose the parameters. Maybe you can choose your units in some way to make some of the parameters disappear?

(d.) Choose a value for the parameter a which generates (from [b]) three steady states. To run your program you will need to chose a value for the discrete time step. Justify your choice, and explain how you will test whether this is a reasonable choice.

(e.) Now run the program, starting at $\tau = 0$ and running out to $\tau = 10$. Try different initial values of $p(\tau = 0)$. In particular, try initial values that are close to the steady state values. Can you verify that two of the steady states are stable, so that if you start near them the solution will evolve toward the steady state? What happens if, in contrast, you start near the unstable state?

Problem 50: As we have noted, the model we have been analyzing is over–simplified. For example, binding of a transcription factor to DNA can't directly change the rate of protein synthesis. Instead, it changes the rate at which mRNA is made, and this in turn changes the rate of protein synthesis. Let's call the mRNA concentration M. Then instead of Eq (2.215) we can write

$$\frac{dM}{dt} = r(F) - k_{\rm RNA} M, \tag{2.233}$$

where $k_{\rm RNA}$ is the rate at which mRNA decays. Then if the rate of protein synthesis is proportional to the mRNA concentration we also have

$$\frac{dP}{dt} = sM - k_{\rm P} P, \tag{2.234}$$

where s is the rate at which one mRNA molecule gets translated into protein and $k_{\rm P}$ is the rate at which the protein decays. Again let's consider a repressor that regulates itself. Then our equations become

$$\begin{aligned} \frac{dM}{dt} &= r_{\max} \frac{F_{1/2}^n}{P^n + F_{1/2}^n} - k_{\rm RNA} M, & (2.235) \\ \frac{dP}{dt} &= sM - k_{\rm P} P, & (2.236) \end{aligned}$$

(a.) Find the conditions for the system to be at a steady state. Reduce your results to a single equation that determines the steady state protein concentration P_0. Does this equation have a single solution or multiple solutions?

(b.) Express the protein concentration as a ratio with $F_{1/2}$, that is $\tilde{P} = P/F_{1/2}$. Can you simplify the steady state condition and show that is only one combination of parameters that determines the value of the steady state $\tilde{P}_0$? Plot the dependence of $\tilde{P}_0$ on this combined parameter.

(c.) Assume that the system is close to the steady state, so that $P = P_0 + \delta P(t)$ and $M = M_0 + \delta M(t)$, with δP and δM small. Find the approximate, linear equations that describe the dynamics of δP and δM.

(d.) Look for solutions of these linear equations in the form $\delta P(t) = Ae^{\lambda t}$ and $\delta M(t) = Be^{\lambda t}$. Show that there is a solution of this form if λ is the solution of a quadratic equation.

(e.) Does the quadratic equation for λ allow for complex solutions? As a hint, try the (admittedly unrealistic) case where the protein and mRNA have the same decay rates, $k_{\rm P} = k_{\rm RNA}$. In contrast, what happens if the mRNA lifetime is very short, that is if $k_{\rm RNA}$ is very large? Explain in words why this system can oscillate, and why these tend to go away if the mRNA is short lived.

Biologically, our simple example of a gene activating itself corresponds to a switch. Given these dynamics, the cell can live happily in two different possible states, one in which the expression of the protein is very low and one it which it is almost as high as it can be. If no extra signals come in from the outside, once a cell picks on of these "valleys," it could (in principle) stay there forever. We can think of this as being a much oversimplified model for differentiation: Two cells, each with exactly the same DNA, can nonetheless adopt two different fates and look to the outside world like two different cells (think again about liver and brain). Alternatively, if our model was describing a single celled organism then the two stable states could represent two very different lifestyles, perhaps appropriate to different environments.

Problem 51: When we discussed simple models for a genetic switch, we considered a protein that could activate its own transcription in a "cooperative" way, so that the rate of protein synthesis was a very steep function of the protein concentration. This actually wouldn't be true if activation depended on the binding of just one molecule to the relevant site along the DNA. Then the synthesis rate would look more like

$$r_{\rm syn}(c) = r_{\rm max}\frac{c}{c+K}, \tag{2.237}$$

where c is the protein concentration, K is a constant, and $r_{\rm max}$ is the maximum rate. The dynamics of c would then be given by

$$\frac{dc}{dt} = r_{\rm syn}(c) - \frac{c}{\tau}, \tag{2.238}$$

where τ is the lifetime of the protein.

(a.) Sketch the behavior of $r_{\rm syn}(c)$. Use this sketch to determine the conditions for a steady state, $dc/dt = 0$. Is there more than one steady state? Does your answer depend on the lifetime τ?

(b.) Are the steady states that you found in [a] stable? This requires a real calculation, not just a sketch.

(c.) Can this system function as a switch? Explain why or why not.

2.5 Stability and oscillation in a real biochemical circuit

The cell cycle is an oscillator. Observations of cells reveal distinct stages of the cell cycle as shown schematically in Figure 2.10. We will consider a modern model[6] for the embryonic cell cycle as a type of "relaxation oscillator." Qualitatively, a relaxation oscillator starts with a bistable system and then adds slow negative feedback that drives the system to switch between the two states. We will review the cell cycle and the model, and finally compare relaxation oscillators to other types of oscillators in light of biological requirements.

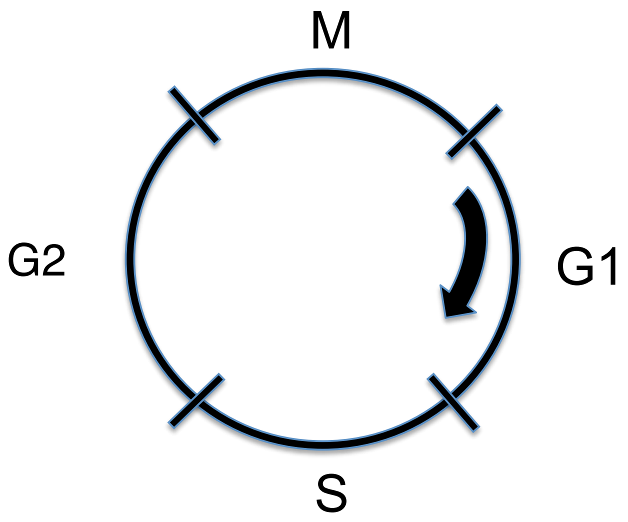


Figure 2.10: Canonical cell cycle. G1 - gap 1, S - DNA synthesis, G2 - gap 2, M - mitosis.

We will consider a simplified model of the embryonic cell cycle of the African clawed frog *Xenopus laevis.* This is a well studied model organism for the cell cycle in part because of the convenience of working with the plentiful and large (~ 1 mm) eggs, and in part because the cytoplasm can be extracted from multiple eggs and used for biochemical studies. After fertilization, the *Xenopus laevis* embryo undergoes exactly twelve rapid (~ 40 minutes), synchronized rounds of cell division. From biochemical studies of extracts, it is found that these cycles will occur in the absence of cells, and even in the absence of DNA! The biochemical network that drives these cy-

---

[6] The discussion here is based largely on JR Pomerening, SY Kim & JE Ferrell, Systems–level dissection of the cell-cycle oscillator: Bypassing positive feedback produces damped oscillations. *Cell* **122,** 565–578 (2005).

cles is shown schematically in Fig 2.11. We read this schematic to mean that Cdk1 activity is increased by dual positive feedbacks (active Cdk1 activates its activator Cdc25 and inactivates its inhibitor Wee1), while Cdk1 activity is reduced by a single negative feedback, in which active Cdk1 activates the anaphase promoting complex (APC). Qualitatively, the system resembles a simple relaxation oscillator in which fast positive feedback leads to two stable states, and slow negative feedback leads to oscillations between these two states. We can capture the essence of their model by considering the Cyclin-Cdk1 complex as an "activator", and APC as a "repressor". The activator rapidly activates its own production and more slowly activates production of the repressor. The repressor eventually builds up and represses production of the activator. The result is an oscillation.

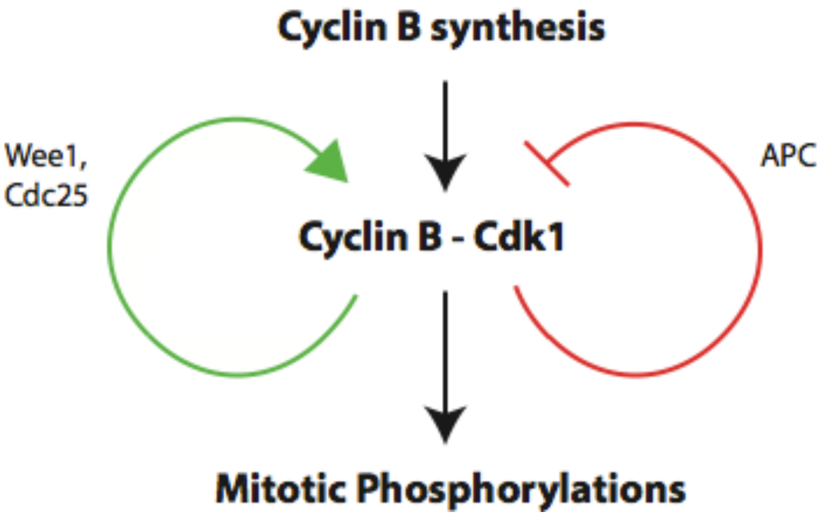


Figure 2.11: The embryonic cell cycle in the African clawed frog *Xenopus laevis* is driven by coupled positive and negative feedback loops.

To understand this system mathematically, let's start with the activator, with no negative feedback. The concentration of activator will increase in time because of production by the cell, and decrease due to degradation:

$$\frac{dA}{dt} = \gamma_0 + \frac{\gamma A^h}{K_A^h + A^h} - \mu A, \qquad h > 1.$$

In addition to the basal rate of production γ_0, the activator increases its own rate of production according to a Hill function with Hill coefficient h. Figure 2.12 shows a schematic example of cooperative gene regulation. The dissociation constant K_A is the concentration of activator at which the regulatory site on the DNA is bound 50% of the time by the activator complex.

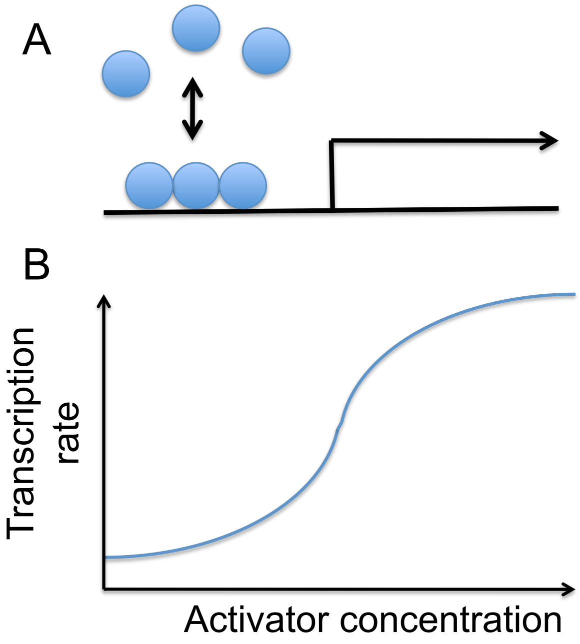


Figure 2.12: Schematic of cooperative gene regulation. (A) If multiple copies of a transcription factor are required to activate (or repress) expression of a gene, then (B) the transcription rate will be a sigmoidal function of the transcription factor concentration, *i.e.* Hill coefficient $h > 1$.

Notice that dA/dt has no explicit dependence on time, so we can plot dA/dt as a function of A, as shown in Fig 2.13. What are the fixed points? What is their stability? To see if a fixed point is stable, examine the sign of

dA/dt on either side of the fixed point. Will small deviations from the fixed point shrink or grow? As plotted in Figure 2.13, the activator is *bistable* and will exhibit hysteresis. That is if the activator A starts out high, it will stay high at the upper fixed point, and if A starts out low it will stay low at the lower fixed point.

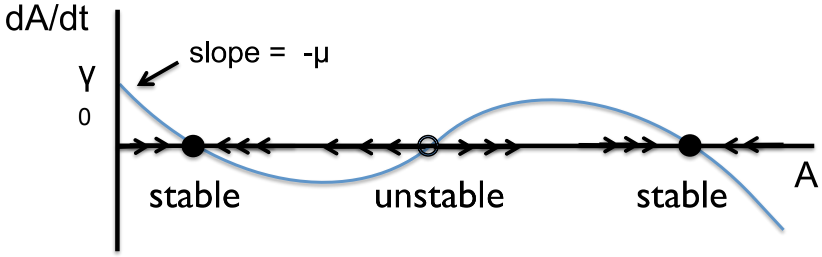


Figure 2.13: Production rate of activator, dA/dt, as a function of the activator concentration A.

Now introduce negative feedback. Specifically, introduce a repressor with concentration R, and let the rate of degradation of A depend on R:

$$\mu \to \mu(R).$$

To be specific, let μ increase linearly with R,

$$\mu(R) = \mu_0 + \beta R.$$

Consider how the dA/dt curve in Fig 2.13 will change as the repressor R concentration changes. The rate of degradation of A will increase, meaning that the linear slope term in dA/dt will get more negative. Eventually this will mean that the upper stable fixed point will disappear. In fact, the upper fixed point will merge with the unstable fixed point – this is called a “saddle-node” bifurcation. (The name makes more sense in two dimensions, imagine a 2D stable fixed point and a 2D saddle-shaped fixed point coming together, yielding no fixed point at all.) With only the lower stable fixed point left, the system will be monostable, *i.e.* whatever initial value of A one starts with, A will steadily change until it reaches its fixed-point value. Similarly, consider starting with the dA/dt curve in Fig 2.13 and letting the repressor concentration R decrease. As the rate of degradation of A decreases, the linear slope term in dA/dt will become less negative. Eventually, the lower stable fixed point will disappear, again by merging with the unstable fixed point in a saddle-node bifurcation, leaving only the upper stable fixed point.

Now, what will happen if the repressor concentration R slowly oscillates between low and high values? The system will start out monostable, say with a low value of A at the only stable fixed point. As R slowly increases, two new fixed points will suddenly appear – an unstable fixed point and an upper stable fixed point. What will happen to the value of A when these new fixed points appear? Nothing! The system will now be bistable, but there's no reason for A to leave the lower stable fixed point. (As long as we don't add any noise to the system...) However, as R keeps increasing, eventually the lower stable fixed point will merge with the unstable fixed point and disappear. Now what happens to the value of A? There's only the upper stable fixed point left, so A will have to jump up to this new, higher value. Then imagine that R starts to decrease. This whole process will repeat itself in reverse. The lower stable fixed point and unstable fixed point will suddenly appear, with nothing happening to the high value of A until the upper stable fixed point merges with the unstable fixed point and disappears, at which point A will jump down to the lower value of the remaining stable fixed point. Slow oscillations of R will therefore lead to a cycle in which A periodically jumps back and forth between low and high values.

How could such an oscillator be implemented by cells? If the rate of change of the repressor concentration dR/dt is made to depend on the value of A, then the oscillator can run by itself. For example, let

$$\frac{dR}{dt} = \frac{\gamma A^{h'}}{K_A^{h'} + A^{h'}} - \mu' R,$$

where the first term is a Hill function with $h' > 1$ and therefore has a sigmoidal shape similar to that shown in Fig 2.12B. With the right choice of parameters, one can have $dR/dt < 0$ when A is at the lower fixed point, and $dR/dt > 0$ when A is at the upper fixed point. This is all that's needed to have the oscillator run by itself. The sigmoidal dependence of dR/dt on A can be implemented by the same kind of cooperative binding of transcription factors to DNA as shown in Fig 2.12A, now with A regulating transcription of the repressor.

This is an example of a “relaxation oscillator”. As promised, we started with a bistable system, and added a slow negative feedback (the repressor) that destabilizes each fixed point in turn, so that the output (the concentration of activator A) jumps back and forth periodically between low and high values. How can one visualize this behavior in a single plot? The answer is the phase portrait shown in Fig 2.14. The axes are the concentrations of activator A and repressor R. If one draws the nullclines, where $dA/dt = 0$ and $dR/dt = 0$, respectively, and draws in a few arrows showing the direction of flow, *i.e.* the direction of the vector $(dA/dt, dR/dt)$, one can qualitatively see how the system behaves. To prove that the fixed point where the nullclines cross is unstable requires a little work, but taking it as given that trajectories cycle away from that point, one can see the form of the relaxation oscillator emerging from the connected series of arrows.

Now we understand the mathematical model for the embryonic cell cycle, but why is this a good way to design an oscillator? For example, why should cells use a relaxation oscillator rather than a simple feedback oscillator? Consider the oscillator shown schematically in Fig 2.15. A constitutively expressed activator that activates its own repressor, with a time delay somewhere in the feedback loop, will typically lead to oscillations. As some parameter is varied, in this case the delay time, the oscillations will first appear with a small amplitude, but finite frequency as shown in the figure. This is called a “Hopf bifurcation”. So this simple feedback oscillator has a tunable amplitude, but approximately fixed frequency. In comparison, a relaxation oscillator has fixed amplitude but tunable frequency, because the underlying bistable system sets the amplitude of the jump in A while the slow build-up of R sets the frequency. Which type of oscillator better matches the requirements of the cell cycle?

2.6 The driven oscillator

We would like to understand what happens when we apply forces to the harmonic oscillator. That is, we want to solve the equation

$$M\frac{d^2x(t)}{dt^2} + \gamma\frac{dx(t)}{dt} + \kappa x(t) = F(t). \tag{2.239}$$

The problem is that, of course, the solution depends on what we choose for the force. It seems natural to ask what happens, but we don’t want to have

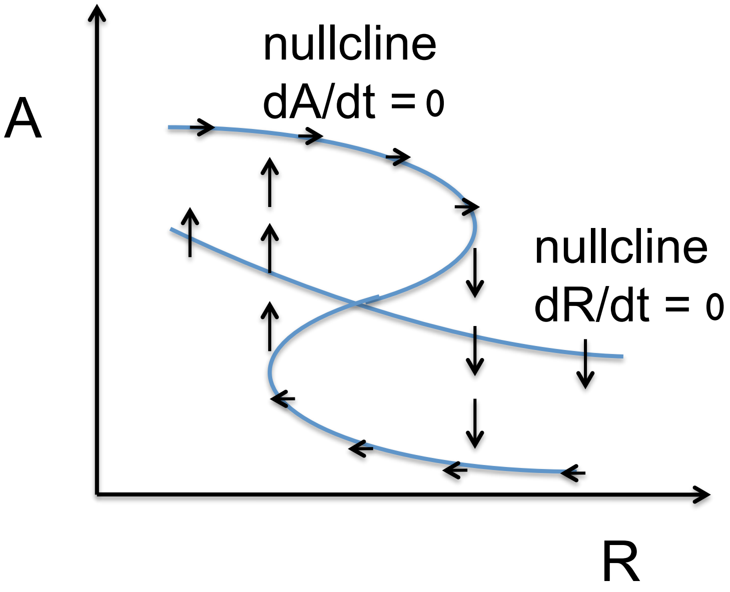


Figure 2.14: Phase portrait of a relaxation oscillator based on an activator A that activates its own production and also activates the production of a repressor R. The repressor feeds back negatively on the activator. All trajectories eventually converge on the same periodic oscillation (indicated by black arrows), with only the phase depending on initial conditions, i.e. this is an example of a "limit cycle oscillator."

to answer with a long list—if the force looks like this, then the displacement looks like that; if the force is different in this way, then the displacement is different in that way ... and so on. Is there any way to give **one** answer to the question of what happens in response to applied forces?

One idea is to think of an arbitrary function $F(t)$ as a sequence of short pules, occurring at the right times with the right amplitudes. This is useful because if we can solve for the response to one pulse, then the response to many pulses is just the sum of the individual responses. To see this, imagine that $x_1(t)$ is the time dependent displacement that is generated by the force

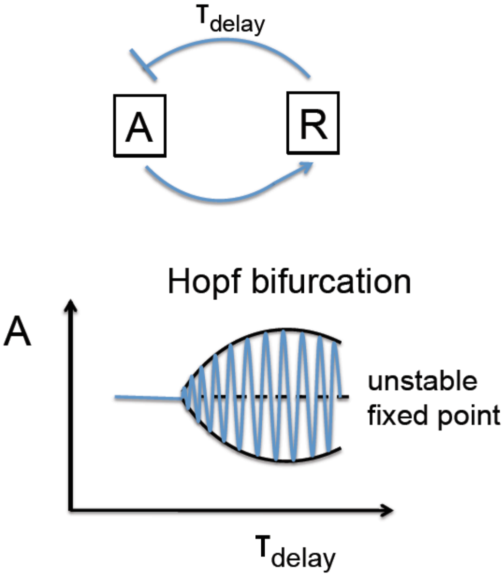


Figure 2.15: Oscillator based on negative feedback with a time delay. Typically, as the time delay increases, the onset of oscillations occurs via a Hopf bifurcation, in this case starting with small, finite frequency oscillations around an unstable fixed point.

$F_1(t)$, and similarly $x_2(t)$ is generated by $F_2(t)$. This means that

$$M\frac{d^2x_1(t)}{dt^2} + \gamma\frac{dx_1(t)}{dt} + \kappa x_1(t) = F_1(t) \tag{2.240}$$

$$M\frac{d^2x_2(t)}{dt^2} + \gamma\frac{dx_2(t)}{dt} + \kappa x_2(t) = F_2(t). \tag{2.241}$$

Now we add these two equations together and notice that adding and diferentiating commute:

$$\begin{aligned}\left[M\frac{d^2x_1(t)}{dt^2} + \gamma\frac{dx_1(t)}{dt} + \kappa x_1(t)\right] &+ \left[M\frac{d^2x_2(t)}{dt^2}\gamma\frac{dx_2(t)}{dt} + \kappa x_2(t)\right] \\ &= F_1(t) + F_2(t) \end{aligned} \tag{2.242}$$

$$\begin{aligned} M\left[\frac{d^2x_1(t)}{dt^2}+\frac{d^2x_2(t)}{dt^2}\right]+\gamma\left[\frac{dx_1(t)}{dt}+\frac{dx_2(t)}{dt}\right] &+ \kappa\left[x_1(t)+x_2(t)\right] \\ &= F_1(t)+F_2(t) \end{aligned} \tag{2.243}$$

$$\begin{aligned} M\frac{d^2[x_1(t)+x_2(t)]}{dt^2}+\gamma\frac{d[x_1(t)+x_2(t)]}{dt} &+ \kappa\left[x_1(t)+x_2(t)\right] \\ &= F_1(t)+F_2(t). \end{aligned} \tag{2.244}$$

Thus if we have the force $F(t) = F_1(t) + F_2(t)$, then the displacement will be $x(t) = x_1(t) + x_2(t)$. This "superposition" of solution keeps working if we have more and more forces to add up, so if we think of the time–dependent force as being a sum of pulses then the displacement will be the sum of responses to the individual pulses, as promised.

Thinking in terms of pulses is a good idea, and we could develop it a little further, but not now.[7] Instead let's look at using sines and cosines (!). Somewhat remarkably, in the same way that we can make an arbitrary function out of many pulses, it turns out that we can make an arbitrary function by adding up sines and cosines. This is surprising because sines and cosines are periodic and extended—how then can we make little localized blips? There is a rigorous theory of all this, but what we need here is just to motivate the idea that sines and cosines are a sensible choice ... .[8]

To understand that sines and cosines can be used to make any function we want, let's try to make a brief pulse. Let's start in a window of time that runs from $t = -10$ up to $t = +10$ (in some units). We can make functions like $\cos(t)$, $\cos(2t)$, and so on. Let's do this in MATLAB, just to be explicit. To do this on a computer we need to discrete time steps, so let's choose steps of size $dt = 0.001$:

```
dt = 0.001;
t = [-10:dt:10];
y= zeros(500,length(t));
for n=1:500;
```

---

[7] We will come back to this in our discussion of waves, starting with the next sections. Stay tuned.

[8] In fact, these ideas will reappear shortly, and then again much later. The idea that we can make arbitrary functions by adding up sines and cosines is called Fourier analysis, and it is an incredibly powerful piece of mathematics, well worth learning properly. Our approach here is a bit haphazard—we take a sort of glancing blow at the material, then circle around for another shot or two before the year is over. We are thinking about a better organization for all of this, but hope you'll bear with us for now.

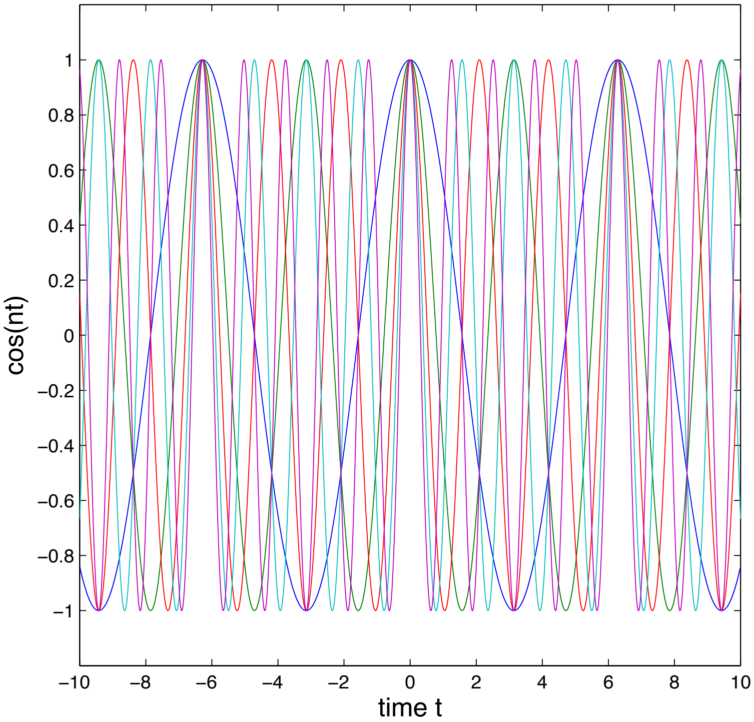


Figure 2.16: The first five members of the family of functions $\cos(nt)$.

```
    y(n,:)  = cos(n*t);
end;
```

This program will generate functions `y(n,t)` $= \cos(nt)$, as shown in Fig 2.16. Notice that all of these functions line up at $t = 0$, where they equal one, and then at other times they have values that have a chance of canceling out.

In fact if we add up all the functions in Fig 2.16, we get the results shown at left in Fig 2.17. If instead of looking at the first five terms, we sum up the first five hundred terms, we get the results shown in Fig 2.17. This should be starting to convince you that we can add up lots of cosines and get something that looks like a perfectly sharp pulse. The only problem is that in addition to a pulse at $t = 0$, we also have pulses at $t = \pm 2\pi$, and if we looked at a bigger window of time we would see pulses at $t = \pm 4\pi$, $t = \pm 6\pi$, etc.. We can start to fix this by including not just $\cos(t)$, $\cos(2t)$, $\cdots$, but also terms like $\cos(1.5t)$, $\cos(2.5t)$, $\cdots$. This will cancel out the pulses at $t = \pm 2\pi$. Then if we add not just halves, but also thirds, fourths, etc we can cancel the pulses at larger and larger times, until eventually all that's left will be the pulse at $t = 0$.

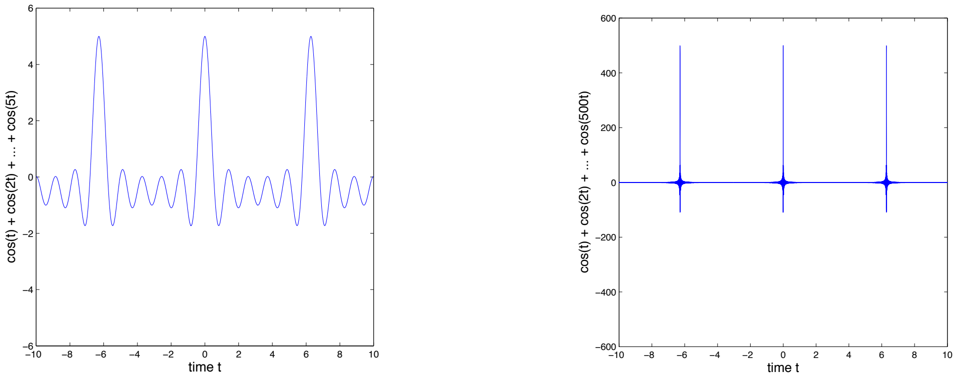


Figure 2.17: Left: The sum of the five functions in Fig 2.16. Right: The sum of five hundred such functions.

The arguments here are not rigorous, but hopefully give the sense that adding up sines and cosines allows us to make pulses. If we can make pulses, we can make anything. Thus any force vs time can be thought of as a sum of sines and cosines. This process is called Fourier analysis, and we'll see more about this in the spring. For now, we know from the discussion above that the displacement in response to this general force can be thought of as the sum of responses to the individual sine and cosine forces. Let's solve *one* of these problems and see how much we can learn.

The problem we want to solve is the damped harmonic oscillator driven by a force that depends on time as a cosine or sine at some frequency ω:

$$M\frac{d^2x(t)}{dt^2} + \gamma\frac{dx(t)}{dt} + \kappa x(t) = F_0\cos(\omega t). \tag{2.245}$$

Actually we might want to do both cosine and sine, and let's call the motion in response to the sine $y(t)$:

$$M\frac{d^2y(t)}{dt^2} + \gamma\frac{dy(t)}{dt} + \kappa y(t) = F_0\sin(\omega t). \tag{2.246}$$

Now these two equations must have the same information hidden in them, since the difference between sine and cosine is just our choice of the point where $t = 0$.

We're going to do something a bit weird, which is to combine the two equations, multiplying the equation for $y(t)$ by a factor of i and then adding the equation for $x(t)$ (!):

$$\begin{aligned} M\frac{d^2x(t)}{dt^2} + \gamma\frac{dx(t)}{dt} + \kappa x(t) &= F_0\cos(\omega t) \\ +i \times \left[M\frac{d^2y(t)}{dt^2} + \gamma\frac{dy(t)}{dt} + \kappa y(t)\right] &= +i \times [F_0\sin(\omega t)] \end{aligned} \tag{2.247}$$

$$\begin{aligned} \Rightarrow M\frac{d^2[x(t)+iy(t)]}{dt^2} + \gamma\frac{d[x(t)+iy(t)]}{dt} &+ \kappa[x(t)+iy(t)] \\ &= F_0[\cos(\omega t) + i\sin(\omega t)]. \end{aligned} \tag{2.248}$$

Now we identify $z(t) = x(t) + iy(t)$, and remember that $\cos(\omega t) + i\sin(\omega t) = \exp(i\omega t)$, so that

$$M\frac{d^2z(t)}{dt^2} + \gamma\frac{dz(t)}{dt} + \kappa z(t) = F_0e^{i\omega t}. \tag{2.249}$$

Notice that the solution to our original physical problem is $x(t) = \text{Re}[z(t)]$.

By now you can anticipate that what we will do is to look for a solution of the form $z(t) = z_0e^{\lambda t}$. As usual this means that $dz/dt = \lambda z_0e^{\lambda t}$ and $d^2z/dt^2 = \lambda^2z_0e^{\lambda t}$. Substituting, we have

$$M\lambda^2z_0e^{\lambda t} + \gamma\lambda z_0e^{\lambda t} + \kappa z_0e^{\lambda t} = F_0e^{i\omega t}. \tag{2.250}$$

Notice that all the terms on the left have a common factor of $z_0e^{\lambda t}$ (this should look familiar!) so we can group them together:

$$\left[M\lambda^2 + \gamma\lambda + \kappa\right] z_0e^{\lambda t} = F_0e^{i\omega t}. \tag{2.251}$$

Now the terms in brackets are just numbers, independent of time. If we want the two sides of the equation to be equal *at all times* then we have to have $e^{\lambda t} = e^{i\omega t}$, or $\lambda = i\omega$. Thus the time dependence of $z(t)$ has to be a complex exponential with the same frequency as the applied force. This means that when we apply a sinusoidal force with frequency ω, the displacement $x(t)$ also will vary as a sine or cosine at with frequency ω.

Once we recognize that $\lambda = i\omega$, we can cancel these exponentials from both sides of the equation and substitute for λ wherever it appears:

$$\begin{aligned}
\left[M\lambda^2+\gamma\lambda+\kappa\right] z_0 e^{\lambda t} &= F_0 e^{i\omega t} \\
\left[M\lambda^2+\gamma\lambda+\kappa\right] z_0 &= F_0 \qquad (2.252)\\
\left[M(i\omega)^2+\gamma(i\omega)+\kappa\right] z_0 &= F_0 \qquad (2.253)\\
\left[-M\omega^2+i\gamma\omega+\kappa\right] z_0 &= F_0 \qquad (2.254)\\
z_0 &= \frac{F_0}{-M\omega^2+i\gamma\omega+\kappa}. \qquad (2.255)
\end{aligned}$$

So we have made it quite far: The position as a function of time $x(t)$ is the real part of $z(t)$, the time dependence is set by $z(t) = z_0 e^{i\omega t}$, and now we have an expression for z_0.

To get a bit further let's recall that, as with any complex number, we can write

$$z_0 = |z_0| e^{i\phi}. \qquad (2.256)$$

Then we have

$$\begin{aligned}
x(t) &= \mathrm{Re}[z(t)] = \mathrm{Re}[z_0 e^{i\omega t}] \qquad (2.257)\\
&= \mathrm{Re}[|z_0| e^{i\phi} e^{i\omega t}] \qquad (2.258)\\
&= \mathrm{Re}[|z_0| e^{i(\omega t+\phi)}] \qquad (2.259)\\
&= |z_0| \cos(\omega t+\phi) \qquad (2.260)
\end{aligned}$$

So we see explicitly that the displacement is a cosine function of time, with an amplitude $|z_0|$ and a phase shift ϕ relative to the driving force. For more on the phase shift see the fourth problem set; for now let's look at the amplitude $|z_0|$.

To compute $|z_0|$ we use the definition $|z| = \sqrt{z^* z}$, where z^* is the complex conjugate of z. Now since F_0 is a real number (it's the actual applied force, and hence a physical quantity!),

$$\begin{aligned}
z_0 &= \frac{F_0}{-M\omega^2+i\gamma\omega+\kappa}\\
\Rightarrow z_0^* &= \frac{F_0}{-M\omega^2-i\gamma\omega+\kappa}. \qquad (2.261)
\end{aligned}$$

Putting these together we have

$$|z_0|^2 = \frac{F_0}{-M\omega^2 + i\gamma\omega + \kappa} \cdot \frac{F_0}{-M\omega^2 - i\gamma\omega + \kappa} \tag{2.262}$$

$$= \frac{F_0^2}{(-M\omega^2 + i\gamma\omega + \kappa)(-M\omega^2 - i\gamma\omega + \kappa)} \tag{2.263}$$

$$= \frac{F_0^2}{(-M\omega^2 + \kappa)^2 + (\gamma\omega)^2}. \tag{2.264}$$

Thus the amplitude of oscillations in response to a force at frequency ω is given by

$$|z_0| = \frac{F_0}{\sqrt{(-M\omega^2 + \kappa)^2 + (\gamma\omega)^2}} \tag{2.265}$$

We see that the amplitude is proportional to the magnitude of the force F_0, which means that the whole system is *linear*; this follows from the fact that the differential equation is linear. Thus it makes sense to measure the coefficient which relates the magnitude of the force to the magnitude of the displacement:

$$G(\omega) \equiv \frac{|z_0|}{F_0} = \frac{1}{\sqrt{(-M\omega^2 + \kappa)^2 + (\gamma\omega)^2}}. \tag{2.266}$$

This is plotted in Fig 2.18, for examples of underdamped and overdamped oscillators. Here we look at some simple limits to get a feeling for how it should behave.

Notice first that at zero frequency we have

$$G(\omega) = \frac{1}{\kappa}. \tag{2.267}$$

This makes sense: zero frequency corresponds to applying a constant force, and if we do this we expect to stretch the spring by a constant amount—since nothing is changing in time mass and drag are irrelevant. The proportionality between force and displacement is the stiffness κ, which appears here as $1/\kappa$ because we ask how much displacement you get for a fixed force, rather than the other way around.

At very high frequencies, the $M\omega^2$ term is bigger than all the others, and so we find

$$G(\omega \to \infty) \approx \frac{1}{M\omega^2}. \tag{2.268}$$

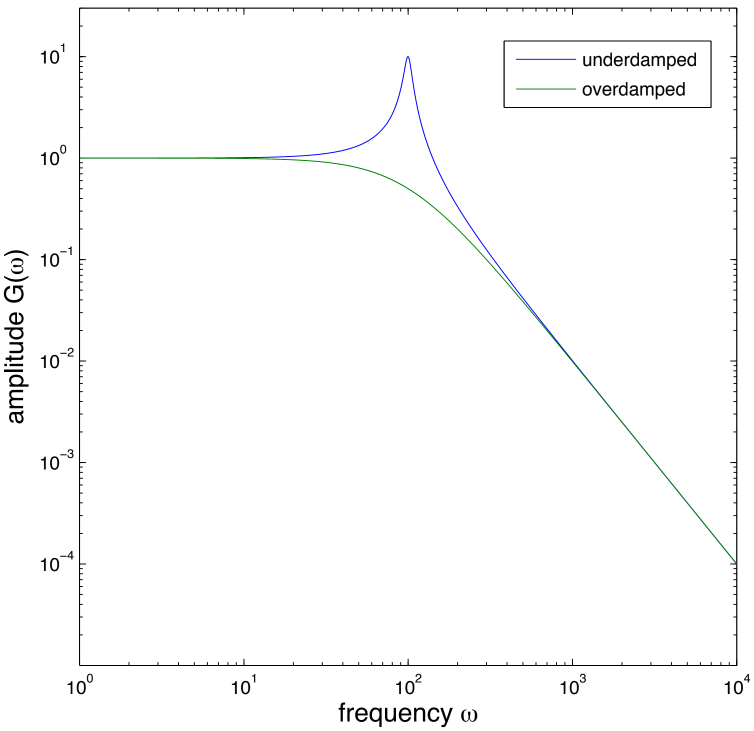


Figure 2.18: Comparing the response $G(\omega)$ for overdamped and underdamped oscillators. In both cases we choose units where $\kappa = 1$ and $\omega_0 = 100$. The underdamped case corresponds to $\gamma = 10$ and the overdamped case $\gamma = 200$. Note the constant behavior $G(\omega \to 0) = 1/\kappa$ at low frequencies, and the asymptotic $G(\omega \to \infty) \approx 1/(M\omega^2)$ at high frequencies. The latter behavior shows up as a line of slope two on this log–log plot.

This actually means that if we are pushing the system at very high frequencies we hardly feel the stiffness or damping at all. What we feel instead is the inertia provided by the mass, and the applied force goes into accelerating this mass.

Finally we notice that, in the denominator of the expression for $G(\omega)$ [Eq (2.266)] there is the combination $(-M\omega^2 + \kappa)^2$. This can never be negative, but it becomes zero when $M\omega^2 = \kappa$, which is the same as $\omega = \omega_0$, where we recall that $\omega_0 = \sqrt{\kappa/M}$ is the natural frequency of the oscillator. Thus when we drive the system with a force that oscillates at the natural frequency, the denominator of $G(\omega)$ can become small, and if γ is small enough this should result in a very large response. This large response is called a *resonance*.

The plot of $G(\omega)$ in Fig 2.18 makes clear how the resonance looks: a peak in the amplitude of oscillations as a function of frequency. What is interesting is that condition for seeing this peak is the same as the condition for underdamping in the motion with no force. Thus the response of the system to applied forces is very closely related to it's "free" decay in the absence of forces. For underdamped oscillators there is a resonant peak and for overdamped oscillators the response just gets smaller as the frequency gets higher, monotonically.

Problem 52: For the driven harmonic oscillator,

$$M\frac{d^2x(t)}{dt^2} + \gamma\frac{dx(t)}{dt} + \kappa x(t) = F(t), \tag{2.269}$$

we showed that if $F(t) = F\cos(\omega t)$, then the position as a function of time can be written as

$$x(t) = \mathrm{Re}[A\exp(i\omega t)], \tag{2.270}$$

where A is given by

$$A = \frac{F}{-M\omega^2 + i\gamma\omega + \kappa}. \tag{2.271}$$

Recall that, as with any complex number, we can write $A = |A|\exp(i\phi_A)$.

(a.) Be sure you understand how to go from Eq (2.271) to the expression for $|A|$, as covered in the lecture. Then derive an expression for ϕ_A, showing explicitly how it depends on the driving frequency ω.

(b.) Does the phase shift ϕ_A have simple behaviors at low frequency ($\omega \to 0$) or at high frequency ($\omega \to \infty$)? Can you give an intuitive explanation for these limiting results?

(c.) Is there anything special about the phase shift at the resonance point where $\omega = \omega_0 = \sqrt{\kappa/M}$? Does this depend on whether the oscillator is underdamped or overdamped?

2.7 Wave phenomena in one dimension

Waves are all around us and can take on many forms. Some are familiar, like the planar waves seen at the beach or the more circular wavefronts observed when you drop a pebble into water. Others, such as the waves that give rise to sound and light, are less obvious to us even though we rely on them constantly. Waves have the amazing ability to transport information and energy across space without actually moving material in the direction of propagation and are the basis for much of the modern technology we take

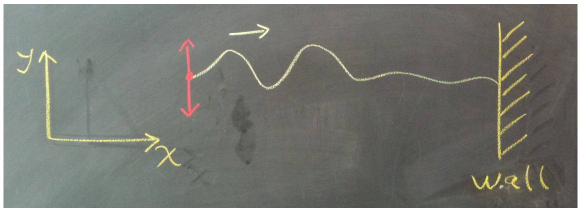


Figure 2.19: A string with one fixed end and one free end. As the end oscillates up and down, a wave will travel down the length of the string.

for granted. In this section, we will explore mechanical waves and save a discussion of light waves for the Spring semester.[9]

We will focus on one special kind of wave, the lateral oscillation of a stretched string such as you might find on a guitar or a piano. The string is a continuous object, so we need more than a simple "coordinate" to describe its configuration at any instance in time. Each infinitesimally small segment of the string has its own position. We need a new concept to describe this—a field. Loosely speaking, a **field** is a quantity that exists everywhere in space and can vary in time. Fields can be **scalars**, like temperature and pressure, or **vectors**, like the gravitational and magnetic fields. For the string, a one–dimensional object, we will have a field, $y(x,t)$ that describes the y–position of the segment of string at position x along the string at time t.

What governs the dynamics of the string? Of course the answer is Newton's Laws, but we need to derive versions of these familiar equations that work on continuous fields. Our strategy will be to apply $F = ma$ to each tiny segment of string along the length and find a consistent solution that allows the string to remain intact.

Let's says the string has a mass M and length L. How much does each of our infinitesimally small segments weigh – what mass do we put in $F = ma$? If the string is homogeneous, so that the material is uniform along its length, then a tiny segment of string with length dx will have a mass

$$m = M\left(\frac{dx}{L}\right) = \left(\frac{M}{L}\right)dx \tag{2.272}$$

The term in parenthesis is the mass of string *per unit length* and we'll call it $\mu \equiv M/L$. So, even though the segment has a vanishingly small size it still has a mass $m = \mu dx$ (which is also vanishingly small!).

Lets say that I pull the string taught by applying a force F to both ends. What happens if you cut the string? My hands fly apart! Of course,

---

[9] In the spring, you will discover that the laws of electromagnetism known as Maxwell's equations lead directly to the wave equation for the propagation of light – one of the true triumphs of physics.

it doesn't matter where along the string you cut it, the same thing will happen.

Figure 2.20: Applying a force to the ends of a string leads to a tension throughout the length.

Now, lets suppose that in the very instance that you cut the string you also grab the two new ends and hold them together. You will need to apply a force of F to each of the new ends in order to balance the force that I am applying to the outer ends. Again, it doesn't matter where along the string you do this, you will need to apply equal and opposite force to each end in order to hold them together.

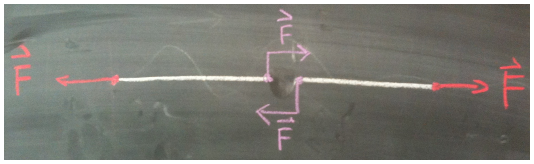


Figure 2.21: The tension in the string is equal to the applied force F.

In fact, before you cut the string, this same force must have existed within the string in order to bind each atom of string to its neighbors. Otherwise the string would move or break because of the lack of force balance. We'll call this force inside the string the **tension**.

Problem 53: A real string will have a bit of elasticity to it and will act like a spring with a large spring constant. If you have a spring, instead of a string, it will stretch if you apply a force to the ends. After it comes to its new equilibrium length, what is the tension in the spring?

The field $y(x,t)$ is a function of two variables, x and t. We'd like to be able to take derivatives of y, for instance to calculate the velocity of the string in the y–direction, but we need to be careful. Let's start by reviewing the concept of a differential of a function $f(x)$ which depends on a single variable. If we change x by a tiny incremental amount dx, then the definition of the first derivative tells us that the function changes by an amount

$$df \equiv \left(\frac{df}{dx}\right) dx \tag{2.273}$$

But what if I told you that $f = ax^2$ and asked you to find df. You would probably say that the derivative of f is $2ax$, making the differential $df = 2ax\,dx$. But why isn't it $x^2\,da$ or maybe the sum of these two things? I know that we have ingrained in you the desire to take derivatives with respect to x and t, but starting now we need to pay a little more attention to the bookkeeping.

To define the differential of a function of more than one variable, we need to introduce the concept of a *partial derivative.* Consider a function $f(x, y)$ which depends on variables x and y. If we keep the variable y fixed and let the variable x change by an amount dx, then f changes by a differential amount

$$df = \left[\lim_{\Delta x \to 0} \frac{f(x + \Delta x, y) - f(x, y)}{\Delta x}\right] dx \tag{2.274}$$

The expression inside the brackets looks like a derivative, but because f is a function of two variables and we are differentiating with respect to only one of them, we call it a partial derivative and denoted it by $\partial f/\partial x$. When you say it aloud, this expression is read "the partial derivative of f with respect to x," or "the partial of f with respect to x." Practically, all you have to do is treat all other variables constant, except the one you are differentiating with.

Consider the function $f(x, y) = x^2 + xy - y^2$ which is shown in Figure 2.22. Using these rules we have

$$\frac{\partial f}{\partial x} = 2x + y \tag{2.275}$$

and

$$\frac{\partial f}{\partial y} = x - 2y \tag{2.276}$$

If you start at point (x, y) and ask how much the function $f(x, y)$ has changed when you move to point $(x + dx, y + dy)$, we can do this in two steps, each time calculating one partial derivative. We first calculate the change

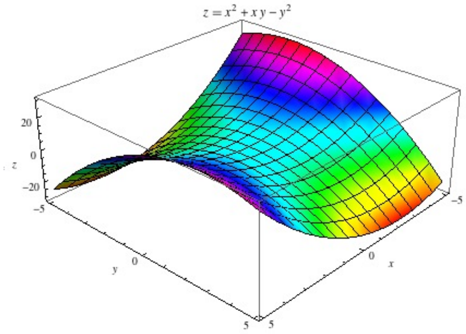


Figure 2.22: A function of two variables.

in f as we go from (x, y) to $(x + dx, y)$ and then add it to the change in f when we go from $(x + dx, y)$ to $(x + dx, y + dy)$ to find the total differential.

$$df \equiv \left(\frac{\partial f}{\partial x}\right) dx + \left(\frac{\partial f}{\partial y}\right) dy \tag{2.277}$$

So, the differential of $f(a, x) = ax^2$ really is $df = 2ax\, dx + x^2\, da$.

Going back to $f(x, y) = x^2 + xy - y^2$, we have four different possible second derivatives:

$$\frac{\partial^2 f}{\partial x^2} = 2 \tag{2.278}$$

$$\frac{\partial^2 f}{\partial x \partial y} = 1 \tag{2.279}$$

$$\frac{\partial^2 f}{\partial y \partial x} = 1 \tag{2.280}$$

$$\frac{\partial^2 f}{\partial y^2} = -2 \tag{2.281}$$

You may have noticed that $\frac{\partial^2 f}{\partial x \partial y} = \frac{\partial^2 f}{\partial y \partial x}$. We won't go through it, but you can show that for any "nice" function, where the function and its derivatives are continuous, the order of differentiation doesn't matter.

Problem 54: If you haven't seen these before you should probably write down a few examples and try them out for yourself.

Let's take a snapshot of the string at time $t = t_0$ as shown in Figure 2.23. We can write $F = ma$ in the y–direction for this tiny segment of string as:

$$F_y = (\mu dx) \times \left(\frac{\partial^2 y(x,t)}{\partial t^2} \right) \tag{2.282}$$

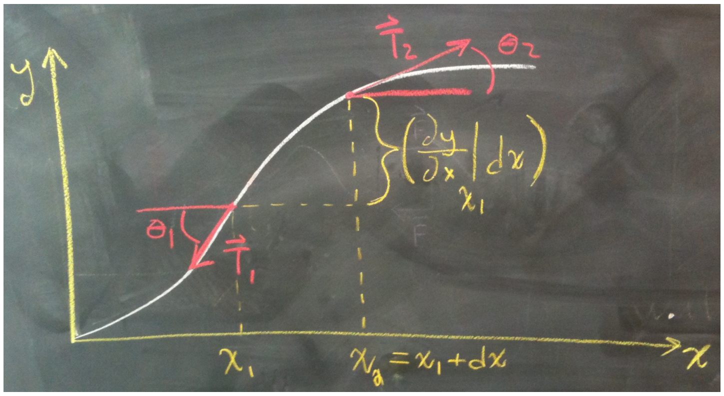


Figure 2.23: The force diagram for a string (shown in red). Note that the tension vector points along the contour of the string, not necessary along the y–direction.

The force in the y–direction is

$$F_y = T\sin\theta_2 - T\sin\theta_1 \tag{2.283}$$

We now make one critical assumption that will make our calculation much easier. We will assume that all the angles are small. For small angles,

$$\sin\theta \approx \tan\theta \tag{2.284}$$

and we can write

$$F_y \approx T\tan\theta_2 - T\tan\theta_1 \tag{2.285}$$

Problem 55: We claimed that Eq (2.284) was valid for "small angles." But, how small is small and when does this approximation start to break down?

(a.) Using MATLAB plot the error in Equation 2.284 as a function of the θ. If you want to define a regime in which the approximation is valid, you need to specify an error that you are willing to live with. For an error of 1%, what is the "threshold" angle above which the approximation can not be used.

(b.) If you go online[10] you can see a high speed video of someone strumming a guitar. Based on an analysis of this video, what is the maximum angle achieved by any local section of guitar string? Is our small angle approximation valid for waves on a guitar string? For your estimated maximum angle, what error does our approximation introduce?

The tangent is the change in y divided by the change in x of the string, i.e. $\tan\theta = \frac{\partial y}{\partial x}$. So, we are left with

$$F_y = T\left[\frac{\partial y(x_2,t)}{\partial x} - \frac{\partial y(x_1,t)}{\partial x}\right] \tag{2.286}$$

As dx becomes smaller and smaller, the term in brackets becomes the second partial derivative evaluated at x_1 times dx:

$$\frac{\partial^2 y(x_1,t)}{\partial x^2} = \frac{d}{dx}\left[\frac{\partial y(x_1,t)}{\partial x}\right] \equiv \frac{\frac{\partial y(x_1+dx,t)}{\partial x} - \frac{\partial y(x_1,t)}{\partial x}}{dx} \tag{2.287}$$

Plugging all this into Equation 2.282, we have

$$T\frac{\partial^2 y(x_1,t)}{\partial x^2}dx = \mu\frac{\partial^2 y(x_1,t)}{\partial t^2}dx \tag{2.288}$$

This looks pretty messy, but we can clean it up by defining a new constant, $c \equiv \sqrt{\frac{T}{\mu}}$. Our results is therefore:

$$\left[\frac{\partial^2}{\partial x^2} - \frac{1}{c^2}\frac{\partial^2}{\partial t^2}\right] y(x,t) = 0 \tag{2.289}$$

This is called the *wave equation* and relates the spatial and temporal derivatives of $y(x,t)$ to each other. It is solutions to this equation that will give rise to many interesting phenomena, including the traveling and standing waves we will study in more detail.

What is c? We can start by calculating its dimensions:

- $[T]$ = Newtons = $\frac{\text{kg m}}{\text{s}^2}$

---

[10] One example is `http://www.guitar-tube.com/watch/high-speed-guitar-video.html`, but you are welcome to find other videos.

- $[\mu] = \frac{\text{mass}}{\text{length}} = \frac{\text{kg}}{\text{m}}$
- $[c] = \sqrt{\frac{\text{kg m/s}^2}{\text{kg/m}}} = \sqrt{\frac{\text{m}^2}{\text{s}^2}} = \frac{\text{m}}{\text{s}}$

So, c is a speed! We will see soon that is the velocity of traveling waves on the string.

What are the solutions of the wave equation? If we choose *any* function $F(x)$ (ok, make it a nice well–defined function...), we will show that $F(x-ct)$ is a solution to Equation 2.289. To start, we need to take derivatives of F with respect to x and t, keeping track of the fact that the argument of F include both x and t.[11]

$$\frac{\partial}{\partial x}F(x-ct) = F'(x-ct) \tag{2.290}$$

$$\frac{\partial^2}{\partial x^2}F(x-ct) = F''(x-ct) \tag{2.291}$$

$$\frac{\partial}{\partial t}F(x-ct) = F'(x-ct)\times(-c) \tag{2.292}$$

$$\frac{\partial^2}{\partial t^2}F(x-ct) = F''(x-ct)\times(c^2) \tag{2.293}$$

Putting Equations 2.291 and 2.293 into Equation 2.289 we find that

$$\left[\frac{\partial^2}{\partial x^2} - \frac{1}{c^2}\frac{\partial^2}{\partial t^2}\right]F(x-ct) = F''(x-ct) - \frac{c^2}{c^2}F''(x-ct) = 0 \tag{2.294}$$

so that $F(x-ct)$ is a solution. You can check for yourself that $F(x+ct)$ will also work. Recall that we didn't specify the shape of F at all, just that the argument of the function was $x-ct$. This will allow us to create many different wave shapes that all travel along the string.

But what does the solution $F(x-ct)$ mean? Consider an arbitrary initial string conformation $y(x,0) = f(x)$. We know that $y(x,t) = f(x-ct)$ will be a solution to the wave equation that retains this initial shape at $t=0$. At a later time, t, the height of the string at position x is $y(x) = f(x-ct)$. Hopefully you can see that the segment of string at position $x' = x - ct$ is at the same y–position at time t as the segment at x was at $t=0$. The waveform has moved a distance ct in time t, i.e. with velocity c. Over time, the waveform retains its shape, but moves to the right at a constant speed c.

---

[11] The prime notation here denotes the derivative with respect to the argument of F, i.e. $' \equiv \frac{\partial}{\partial \mathbb{X}}$, where in this case $\mathbb{X} = x - ct$.

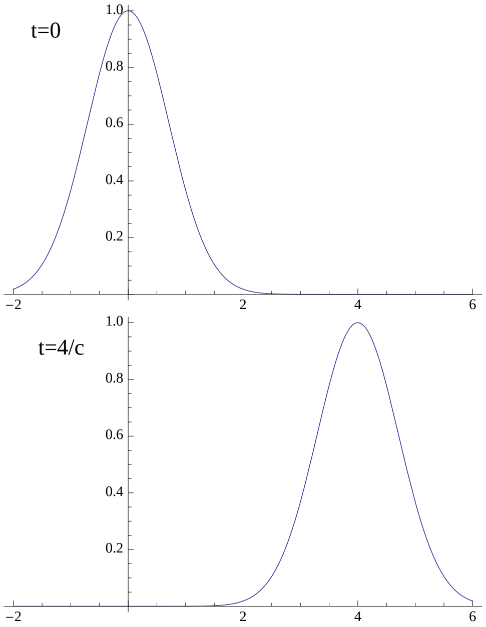


Figure 2.24: A gaussian wave propagating in the $+x$–direction.

Let's work out the specific example of a moving gaussian wave. Let

$$y(x,t) = e^{-(x-ct)^2} \tag{2.295}$$

a gaussian centered at $x = ct$. Note, that the shape (e.g. the width) does not change over time, but the whole shape moves to the right with speed c as shown in Figure 2.24. It is worth reiterating that the string isn't moving in the x–direction, but the "wave" is. It moves at speed c and can carry energy in the x–direction. But, the string is only moving in the y–direction. This might seem a little puzzling. How can you transmit energy in a direction that is different the direction of motion of the actual mass? It all relies on the tension and the binding energy of each segment of string to its neighbors.

The velocity in the y–direction of the string is found by taking the derivative of Equation 2.295

$$v_y = \frac{\partial y}{\partial t} = 2c(x-ct)e^{-(x-ct)^2} \tag{2.296}$$

Does this make sense? As the gaussian shape moves to the right, the left

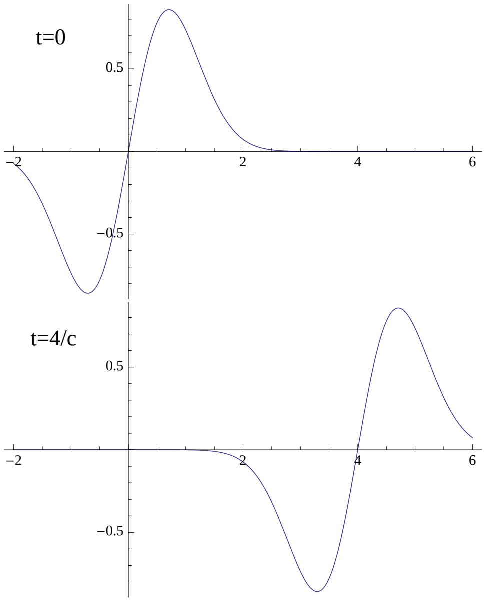


Figure 2.25: The y–velocity of the gaussian wave packet at two different times.

side of the curve must move down and the right side must move up as shown in Figures 2.25 and 2.26.

Because the wave equation is made of simple derivatives, if $F(x,t)$ and $G(x,t)$ are solutions, then so is their sum $F(x,t)+G(x,t)$. You can easily check that when you put this in the wave equation all the terms produce simple sums and you essentially get two wave equations which both evaluate to zero. We will find it useful in several instances to combine a left–ward and a right–ward moving wave

$$y(x,t) = F(x-ct) + G(x+ct) \tag{2.297}$$

What happens when a wave reaches the end of a string? It depends on the boundary conditions you've setup. Consider first the case of a string whose end at $x=0$ is physical restrained so that $y(0,t)=0$ for all time. When a wave hits the end you will get a reflected wave that comes out traveling in the opposite direction.

What makes the reflected wave? The force at the fixed end is generated by the attachment (by you if you're holding the string). As the input wave reaches the fixed point, it applies an upward force. You then have to apply

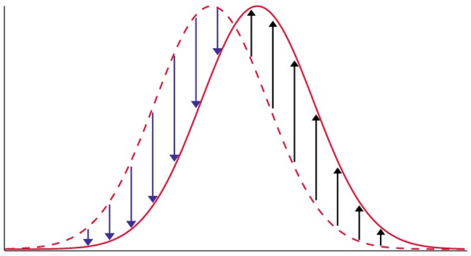


Figure 2.26: Conceptual picture of the gaussian wave packet velocity.

an equal force in the downward direction in order to keep the end fixed. This applied force changes over time as the incoming wave hits the origin. *This* is what generates the reflected wave which is flipped over compared to the incoming wave (you pull down when the string is pulling up).

What does the reflected wave look like? Well, we just argued that it should look something like the input wave with a negative amplitude. Mathematically, we can satisfy our boundary condition by making our final solution a superposition of the original incoming wave and another wave, the reflected one, that exactly cancels out the incoming wave at $x = 0$. In other words, we are looking for a solution $y(x,t) = F_{incoming}(x,t) + G_{reflected}(x,t)$ that does this. We will assume our incoming wave is moving leftward towards the origin, so that

$$F_{incoming}(x,t) = F(x + ct) \tag{2.298}$$

where $F(x)$ is *any* well–behaved function. In order to satisfy the boundary condition, all we have to do is set

$$G_{reflected}(x,t) = -F(-x + ct) \tag{2.299}$$

Because the argument of the functions looks like $x - ct$, they satisfy the wave equation, and at $x = 0$

$$y(0,t) = F(ct) - F(ct) = 0 \tag{2.300}$$

for all times as shown in Figure 2.27.[12]

---

[12] This solution has values for $x < 0$, where there is no string. It might help to visualize an "imaginary" world to the left of the origin in which the two waves can travel. But you know that in reality the forces generated at the attachment point create the reflected wave.

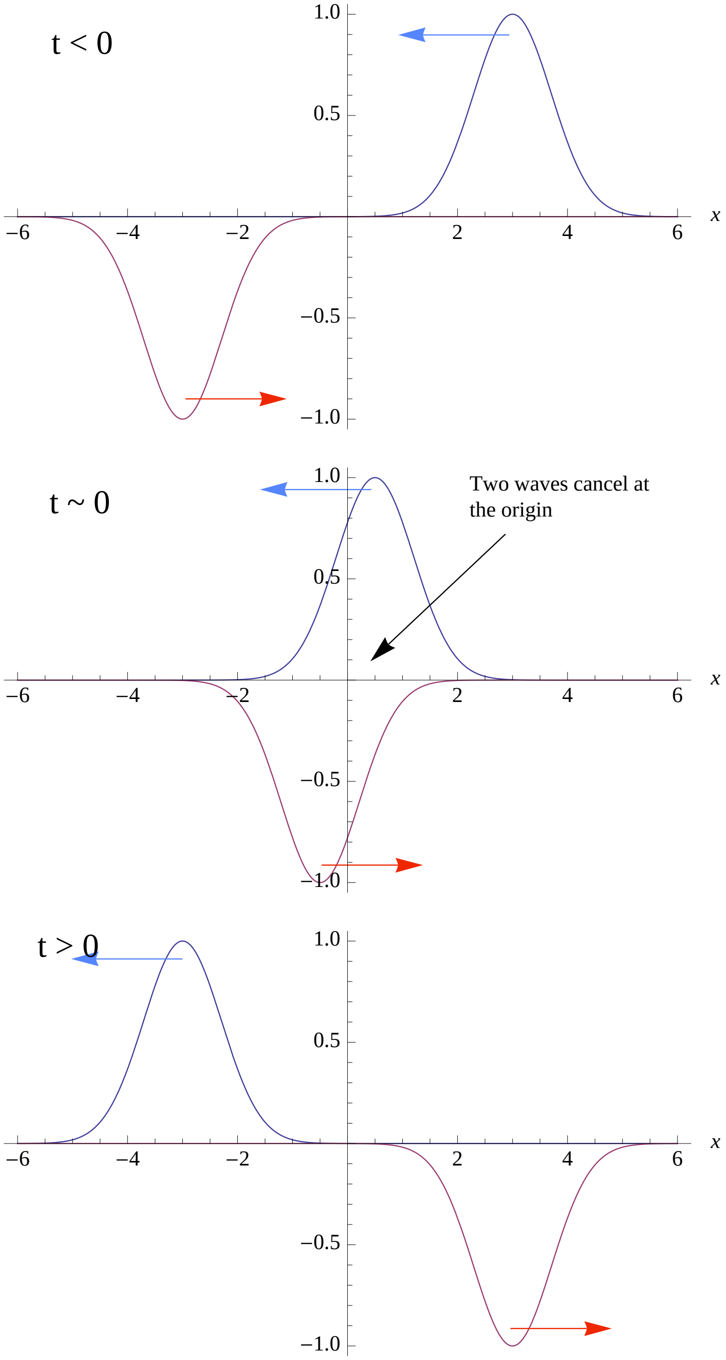


Figure 2.27: The motion of the incoming (blue) and reflected (red) waves for a fixed–end string.

Now lets send a wave down a string in which one end is fixed at $x = 0$ but is free to move in the y–direction. You can create something like this by imagining the end of the string is attached to a frictionless ring that moves along a rod at $x = 0$ as shown in Figure 2.28.

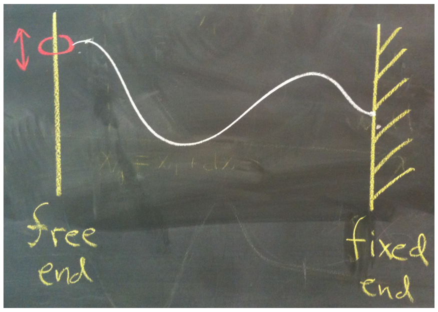


Figure 2.28: A string with a "free" end at $x = 0$.

In this case, the boundary condition is that the derivative of y with respect to x has to be zero at the origin for all time. So, we have

$$\left.\frac{\partial y(x,t)}{\partial x}\right|_{x=0} = 0 \tag{2.301}$$

In this case the solution is $y(x,t) = F(x+ct) + F(-x+ct)$ so that the reflected wave amplitude has the same sign as the incoming wave and is not flipped over. Lets check that this satisfies the boundary conditions.

$$\begin{aligned}
y(x,t) &= F(x+ct) + F(-x+ct) && (2.302)\\
y(0,t) &= 2F(ct) && (2.303)\\
\left.\frac{\partial y(x,t)}{\partial x}\right|_{x=0} &= F'(x+ct) + -1 * F'(-x+ct)\Big|_{x=0} && (2.304)\\
&= F'(ct) - F'(ct) = 0 \quad \checkmark && (2.305)
\end{aligned}$$

Note that in this case the end moves over time.

Consider the following sinusoidal waveform with amplitude A and wavelength λ that travels to the right along the x–axis:

$$y(x,t) = A\sin\left[\frac{2\pi}{\lambda}(x-ct)\right] \tag{2.306}$$

The wave obviously transfers energy along the x–axis. But what is each bit of string doing? If we look at the y–position of a piece of string at position $x = 0$ we find:

$$y_0(t) = -A\sin\frac{2\pi ct}{\lambda} \tag{2.307}$$

The piece moves harmonically in time. As the wave moves to the right, each piece of string continually goes up and down in a sinusoidal pattern in *time*. It is also worth noting that if we chose a piece of string at a different position along the x–axis, the motion will be the same except for a phase shift. The amplitude of the motion of each piece doesn't depend on x.

There's another set of solutions to the wave equation in which the wave amplitude but not the shape depends on time. We will call these waves "standing waves." The fact that the shape doesn't depend on time means that we can separate the x and t variables in our solution:

$$y(x,t) = f(x)g(t) \tag{2.308}$$

The shape of the waveform is given by the function $f(x)$ and doesn't change with time. But the amplitude is given by $g(t)$, which does change over time. In particular, if $f(x_0) = 0$ for some point x_0, then $y(x_0,t) = 0$ for all times. This type of point in a wave, where there is no motion, is called a *node* and it will be important in our thinking about musical instruments.

Putting this into the wave equation we get:

$$\left(\frac{\partial^2}{\partial x^2} - \frac{1}{c^2}\frac{\partial^2}{\partial t^2}\right) f(x)g(t) = \frac{\partial^2 f(x)}{\partial x^2} g(t) - \frac{1}{c^2}\frac{\partial^2 g(t)}{\partial t^2} f(x) = 0 \tag{2.309}$$

We can rearrange Equation 2.309 to find an equation that relates terms with $f(x)$'s in them to terms with $g(t)$'s in them.

$$\frac{\frac{\partial^2 f(x)}{\partial x^2}}{f(x)} = \frac{1}{c^2}\frac{\frac{\partial^2 g(t)}{\partial t^2}}{g(t)} \tag{2.310}$$

This equation must be true for *any* particular $f(x)$ and $g(t)$. The only way this can work out is if each side of Equation 2.310 is equal to a constant that doesn't depend on your choice of $f(x)$ or $g(t)$. We will call this constant k^2 (the meaning of k will become apparent in a bit). We now have two differential equations which separately govern the behavior of $f(x)$ and $g(t)$:

$$\frac{\partial^2 f(x)}{\partial x^2} + k^2 f(x) = 0 \tag{2.311}$$

$$\frac{\partial^2 g(t)}{\partial t^2} + k^2c^2 g(t) = 0 \tag{2.312}$$

You've seen these second–order equations before and they have solutions:

$$f(x) = A\cos(kx) \tag{2.313}$$

$$g(t) = A\cos(\omega t) \tag{2.314}$$

where $\omega \equiv kc$. In order to satisfy the wave equation and retain the separation of variables, both the spatial wave shape and the temporal wave amplitude must be harmonic.

Our general solution is therefore

$$y(x,t) = A\cos(kx)\cos(\omega t) \tag{2.315}$$

Now we see that the constant k is the spatial angular frequency of the harmonic wave shape. It is traditionally called the **wave number**. ω is the temporal angular frequency of the wave amplitude. We can relate these to some more familiar quantities, the wavelength λ and the frequency ν:

$$k \equiv \frac{2\pi}{\lambda} \tag{2.316}$$

$$\omega \equiv 2\pi\nu \tag{2.317}$$

Why is this called a wave? Unlike the traveling wave solutions from before, there doesn't seem to be any motion along the x–axis in this solution. We can rewrite Equation 2.315 to recover terms that look like our $F(x-ct)$ solutions:

$$\begin{aligned} y(x,t) &= A\cos(kx)\cos(\omega t) && (2.318)\\ &= \frac{A}{2}\cos(kx+\omega t) + \frac{A}{2}\cos(kx-\omega t) && (2.319)\\ &= \frac{A}{2}\cos\left[k(x+ct)\right] + \frac{A}{2}\cos\left[k(x-ct)\right] && (2.320) \end{aligned}$$

The standing wave solution is just the superposition of a left–moving and a right–moving traveling wave. Figure 2.29 may help you visualize this.

2.8 More about 1D waves

Musical instruments like the guitar, violin, hammer dulcimer, piano, harpsichord etc. use standing waves on strings with two fixed ends to produce tones of a certain pitch. Lets now fix both ends of a string and ask what kind of standing wave solutions we get.

The boundary condition is that the lateral displacement at each end must be zero, i.e. $y(0,t) = y(L,t) = 0$. We will look for standing wave solutions where we can separate the spatial and temporal wave functions $y(x,t) = f(x)g(t)$ that satify this condition, i.e. where $f(0) = f(L) = 0$.

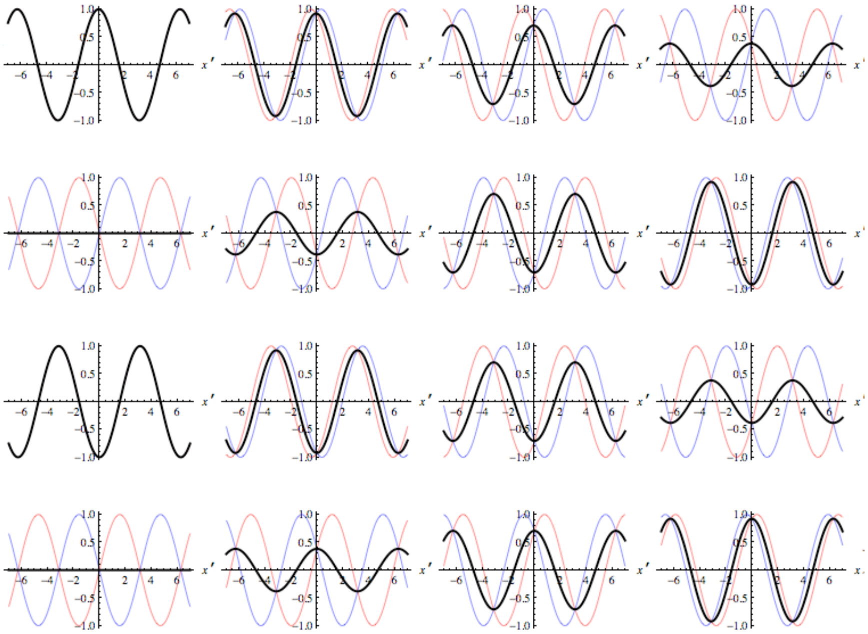


Figure 2.29: Snapshots of two oppositely directed traveling waves (red and bludrope) and their sum (black, a standing wave) over time. $t = 0$ is at the upper left and the time moves to the right and then down.

Our standing wave solution from equation 2.313 was completely general, and we just have to find which of these sinusoidal functions satisfies the boundary condition. If $f(x) = \sin(kx)$, then we have

$$f(0) = \sin(0) = 0 \quad \checkmark \tag{2.321}$$
$$f(L) = \sin(kL) = 0 \tag{2.322}$$

Equation 2.322 is only satisfied if $kL = \pi, 2\pi, 3\pi, \ldots$, an integer multiple of π. In other words, only a discrete, but infinite, number of wave numbers will give rise to standing waves on our string.

$$k = \frac{n\pi}{L}; \quad n \in \mathbb{Z} \tag{2.323}$$

Our solution now becomes

$$y_n(x,t) = A_n \sin\left(\frac{n\pi}{L}x\right)\cos\left(\frac{n\pi c}{L}t\right) \tag{2.324}$$

Each of these "modes," denoted by n, vibrates with a different temporal frequency that increases linearly with n. The first three mode shapes are shown in Figure 2.30.

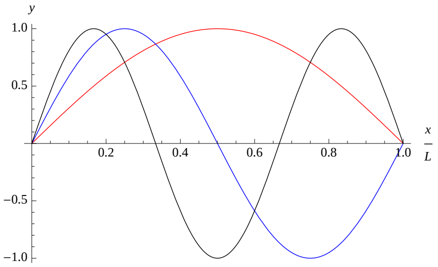


Figure 2.30: Standing wave solutions on a end–fixed string for $n = 1$ (red), $n = 2$ (blue) and $n = 3$ (black). Note that there is no "node" for $n = 1$, but one and two nodes for $n = 2, 3$.

The number of *nodes* in each *mode* is important for musical instruments.[13] You may know that if you pluck a guitar and hold your finger at exactly the midpoint of the string you can get a "harmonic," a tone that is twice the pitch of the unperturbed string. What you are doing in this case is forcing the existence of a node at the position of your finger. The fundamental mode has a lot of amplitude at that point where the string can't vibrate. But the $n = 2$ mode has a node in the middle and your finger causes this mode to be excited. The frequency of this mode is twice as high

---

[13] ... and extremely important for quantum mechanics and quantum chemistry as you will learn in the Spring.

as the $n = 1$ mode and that is why you hear an octave tone. If you now push your finger down to fret the note at the middle position you hear the same high tone. In this case, you are exciting the $n = 1$ mode but you've shortened the length by a factor of two which gives the same frequency

$$\text{(Fundamental) } n = 1, L = \frac{L'}{2}; \quad \omega = \frac{1\pi c}{\frac{L'}{2}} = \frac{2\pi c}{L'} \tag{2.325}$$

$$\text{(1st Harmonic) } n = 2, L = L'; \quad \omega = \frac{2\pi c}{L'} \tag{2.326}$$

You may recall that the wave speed was related to the tension in the string and the mass per unit length, $c = \sqrt{\frac{T}{\mu}}$. The frequency of vibration is therefore

$$\nu = \frac{n}{2L}\sqrt{\frac{T}{\mu}} \tag{2.327}$$

If you examine the strings on an instrument, you'll see that the higher the pitch, the thinner the string and thus the lower the mass per unit length because $\nu \sim \mu^{-1/2}$. In order to tune the frequency of an individual string, you change the tension and use the fact that $\nu \sim T^{1/2}$.

Problem 56: A organ pipe also uses standing sound waves of air vibrations inside the pipes to produce musical notes. The bottom of the pipe is closed and the air can't move there but the top of the pipe is open and the air can move. You will model this by thinking about waves on a string and assuming a mixed boundary condition where one end of the string is fixed and the other is free to move in the y–direction as discussed above.

(a.) What are the standing wave solutions that you get in this case?

(b.) For the pipe organ, what are the relevant analogs of the tension and the mass per unit length? How would you go about tuning a pipe organ?

You should be a little concerned about our discussion of strumming a guitar string. When you hit the string to strum it, the string shape certainly doesn't look like the perfect sine waves we found as the standing wave solutions. What happens to the string and how can we relate it to the standing waves? To start, we will assume that we have a string with two fixed ends and start the wave with an initial shape $u(x)$ and y–velocity $v(x)$, i.e.

$$y(x,0) = u(x) \tag{2.328}$$

$$\left.\frac{\partial}{\partial t} y(x,t)\right|_{t=0} = v(x) \tag{2.329}$$

Key math concept: What we need to do now is write the initial waveform as a superposition of the different standing wave solutions – the sines and cosines. You already know that *any* arbitrary function can be written as a sum of polynomials in a Taylor's series. When we discussed the driven oscillator, we also claimed that any periodic function could be written as a sum of sines and cosines, which was first shown by the French mathematician J. Fourier (1768–1830) [14]

$$f(x) = A_0 + \sum_n \left[A_n \sin(nkx) + B_n \cos(nkx)\right] \tag{2.330}$$

where $k = \frac{2\pi}{\lambda}$ is the wave number associated with the wavelength of $f(x)$.

Since the ends of our string are fixed, we have nodes at $x = 0, L$ and we can consider L to be our period. The fixed end at $x = 0$ implies that we can't have any of the cosine terms from Equation 2.330. We can therefore write the general standing wave solution as

$$y(x,t) = \sum_n \left[A_n \sin(k_n ct) + B_n \cos(k_n ct)\right] \sin(k_n x) \tag{2.331}$$

where $k_n = \frac{n\pi}{L}$. We have kept both the sine and cosine terms in time to allow us to match any initial condition.

Lets look at this more carefully now. Each of the terms of the sum in Equation 2.331 is a standing wave solution to the wave equation that obeys the fixed–end boundary conditions. Our task is to find the different coefficients A_n and B_n such that $y(x,t)$ matches our initial conditions described by $u(x)$ and $v(x)$.

$$u(x) = y(x,0) = \sum_n B_n \sin\left(\frac{n\pi x}{L}\right) \tag{2.332}$$

$$v(x) = \left.\frac{\partial y(x,t)}{\partial t}\right|_{t=0} = \sum_n A_n \left(\frac{n\pi x}{L}\right) \sin\left(\frac{n\pi x}{L}\right) \tag{2.333}$$

---

[14] If the function is not periodic, the sum is replaced with an integral in what is called a Fourier Transform. You'll return to this topic in the Spring semester.

What are the correct A's and B's that will make Equations 2.332 and 2.333 work out? To find them we first need to introduce a few mathematical formulas:

$$\int_0^L \sin\left(\frac{n\pi x}{L}\right)\sin\left(\frac{m\pi x}{L}\right) = \frac{L}{2}\delta_{nm} \tag{2.334}$$

$$\int_0^L \cos\left(\frac{n\pi x}{L}\right)\cos\left(\frac{m\pi x}{L}\right) = \frac{L}{2}\delta_{nm} \tag{2.335}$$

$$\int_0^L \sin\left(\frac{n\pi x}{L}\right)\cos\left(\frac{m\pi x}{L}\right) = 0; \quad \text{for all } n, m \tag{2.336}$$

The function δ_{nm} is the Kronecker delta function, named after Leopold Kronecker (1823-1891), which is defined as

$$\delta_{nm} = \begin{cases} 1, & \text{if} \quad n = m \\ 0, & \text{if} \quad n \neq m \end{cases} \tag{2.337}$$

With these formulas in hand, we can now calculate the appropriate coefficients. The key is that if we want to pick out how much of the amplitude in a function $f(x)$ is described by a particular sine–function with wave number k, we just need to calculate the integral of $f(x)$ times $\sin(kx)$. The δ–function takes care of removing all the amplitudes that don't match our particular wave number.[15]

Problem 57: Check Equations 2.334, 2.335 and 2.336 for $(n, m) = (1, 1)$ and $(n, m) = (1, 2)$.

This will probably be clearer if we just calculate the coefficients. Lets start by integrating $\sin\left(\frac{n\pi x}{L}\right)$ times $u(x)$, using our result from Equation 2.332:

---

[15] This might seem something like a dot–product from vector geometry and it is! We usually describe a vector, $\mathbf{v}$, in 3–dimensional space by listing the components of the vector along some set of axes (v_x, v_y, v_z). To find a particular component of the vector, you take the dot product along the direction of interest: $v_x = \mathbf{v} \cdot \hat{x}$. Here, we are describing a function $f(x)$ in a space of sine–waves described by components $(A_1, B_1, A_2, B_2, \ldots)$. In order to find a particular component we take the integral of the function with a sine or cosine function with the wave number of interest: $A_1 = \int f(x) \sin(k_1 x) dx$.

$$\int_0^L dx \sin\left(\frac{n\pi x}{L}\right) u(x) = \int_0^L dx \sin\left(\frac{n\pi x}{L}\right)\left[\sum_m B_m \sin\left(\frac{m\pi x}{L}\right)\right] \tag{2.338}$$

$$= \sum_m B_m \left[\int_0^L dx \sin\left(\frac{n\pi x}{L}\right)\sin\left(\frac{m\pi x}{L}\right)\right] \tag{2.339}$$

$$= \sum_m B_m \left(\frac{L}{2}\right)\delta_{nm} \tag{2.340}$$

$$= \frac{L}{2}B_n \tag{2.341}$$

We can do the same with $v(x)$:

$$\int_0^L dx \sin\left(\frac{n\pi x}{L}\right) v(x) = \int_0^L dx \sin\left(\frac{n\pi x}{L}\right)\left[\sum_m \frac{m\pi c}{L} A_m \sin\left(\frac{m\pi x}{L}\right)\right] \tag{2.342}$$

$$= \sum_m \frac{m\pi c}{L} A_m \left[\int_0^L dx \sin\left(\frac{n\pi x}{L}\right)\sin\left(\frac{m\pi x}{L}\right)\right] \tag{2.343}$$

$$= \sum_m \frac{m\pi c}{L} A_m \left(\frac{L}{2}\right)\delta_{nm} \tag{2.344}$$

$$= \frac{L}{2}\frac{n\pi c}{L}A_n = \frac{n\pi c}{2}A_n \tag{2.345}$$

So, thats it. Equations 2.341 and 2.345 allow us to calculate the coefficients A_n and B_n from our initial conditions $u(x)$ and $v(x)$:

$$A_n = \frac{2}{n\pi c}\int_0^L \sin\left(\frac{n\pi x}{L}\right) v(x)dx \tag{2.346}$$

$$B_n = \frac{2}{L}\int_0^L \sin\left(\frac{n\pi x}{L}\right) u(x)dx \tag{2.347}$$

Problem 58: In this problem you'll think about the standing wave produced when you pluck a string on a guitar. As you let go of the string it starts as an approximately triangular shape at rest. Our initial conditions are:

$$u(x) = \begin{cases} x/L, & \text{if} \quad 0 \leq x \leq L/2 \\ 1 - x/L, & \text{if} \quad L/2 \leq x \leq L \end{cases} \tag{2.348}$$

$$v(x) = 0 \tag{2.349}$$

(a.) Sketch the initial shape of the waveform.

(b.) Calculate the Fourier amplitudes A_n and B_n that satisfy the initial conditions.

(c.) How fast does each of the n modes vibrate? Do you hear all these "notes"?

(d.) You've seen that friction is proportional to velocity. In general, the dissipation of energy in the vibrating string is also proportional to velocity. Using this fact, describe in words what happens to all the modes after you pluck the string. What consequence does this have for the perceived "note" that is played when you pluck the string?

Chapter 3

The conservation of energy

So far in this course we have used Newton's laws to solve the dynamics of a number of specific systems by writing these laws as differential equations, $v = \frac{dx}{dt}$ and $F = m\frac{d^2x}{dt^2}$. If we know the starting position and velocity of an object, we can then use the velocity and force to update these quantities iteratively over time. In fact, this is exactly how one solves these types of differential equations numerically on a computer, by moving incrementally in *dt*–sized time steps. In some sense, we can think of Newton's laws as "local" in time in that they tell us how to go from one point in time to the next.

But there are other kinds of statements that we can make about a physical system that are not local in time. These include the idea that the earth revolves around the sun and that a mass on a spring will go up and down over and over. The term "goes around the sun" is most certainly not a local statement because if you watch the system at any one time you only see it move by one time step and can't see that the orbit of the earth is an ellipse and that it even closes on itself and will continue in the same orbit. These statements are more "global" and they describe not just how the system goes from time point to time point, but rather how the system will behave forever.

Another kind of global statement comes in the form of *conservation laws*, which state that a particular measurable property of a system remains constant in time, even as the system evolves. Examples include the conservation of energy and momentum which you have probably seen before. One truly beautiful concept that arose in the early 20th century is called *Noether's Theorem*, which draws a one–to–one correspondence between symmetries in nature and conservation laws. As an example of this, we will see later on that the conservation of momentum is true even when Newton's laws don't hold, e.g. in Quantum Mechanics, and that this law is related directly to the fact that physical systems behave the same regardless of how they are positioned in space.

3.1 Kinetic and potential energies

Let's start by supposing that the force on an object is a function of the position of the object in space but not on the velocity or time so that we can write

$$m\frac{dx^2}{dt^2} = F(x) \tag{3.1}$$

The familiar example of a mass on a spring, $F(x) = -kx$, is just one example. We will now look for a quantity, E, that remains fixed in time so that $dE/dt = 0$. This constant may depend on the position and/or velocity of the object so that $E(x, v)$ is a function of two variables. We can write the total differential of E as

$$dE(x,v) = \left[\frac{\partial E(x,v)}{\partial x}\right] dx + \left[\frac{\partial E(x,v)}{\partial v}\right] dv \tag{3.2}$$

The condition that E remain constant in time then becomes

$$\frac{dE(x,v)}{dt} = \left[\frac{\partial E(x,v)}{\partial x}\right] \frac{dx}{dt} + \left[\frac{\partial E(x,v)}{\partial v}\right] \frac{dv}{dt} = 0 \tag{3.3}$$

which can be rewritten as

$$\left[\frac{\partial E(x,v)}{\partial v}\right] \frac{dv}{dt} = -\left[\frac{\partial E(x,v)}{\partial x}\right] \frac{dx}{dt} \tag{3.4}$$

Now, if we multiply Equation 3.1 by dx/dt, we find that

$$\left[m\frac{dx}{dt}\right] \frac{dv}{dt} = \left[F(x)\right] \frac{dx}{dt} \tag{3.5}$$

Comparing the two previous equations, we see that they look quite similar. If we can find a form for $E(x, v)$ such that the terms in brackets on each side of the equations are equal, then we will have found our constant of the motion. This procedure produces two equations for $E(x, v)$

$$\frac{\partial E(x,v)}{\partial v} = m\frac{dx}{dt} = mv \tag{3.6}$$

$$-\frac{\partial E(x,v)}{\partial x} = F(x) \tag{3.7}$$

In general, this looks like it might be messy, but it isn't because each equation above only depends on x or v, but not both. When we integrate equation 3.6 with respect to v, the constant of integration will not depend on v, but can depend on x. Equation 3.6 therefore requires that

$$E(x,v) = \frac{1}{2}mv^2 + g(x) \tag{3.8}$$

where $g(x)$ is the "constant" of integration. Likewise, integration of equation 3.7 yields [1]

$$E(x,v) = -\int_0^x F(x')dx' + h(v) \tag{3.9}$$

Because of the separation of variables in these two equations, both will be satisfied if we write

$$E(x,v) = \frac{1}{2}mv^2 - \int_0^x F(x')dx' \tag{3.10}$$

So thats it. Newton's second law guarantees that E, which we can now identify as the total energy, remains constant as the system evolves in time. In fact, Newton's equations are equivalent to the statement that the total energy remains constant along a particle's trajectory.

The first term in the energy is related to the motion of the particle and we call this the *kinetic energy*, $K = \frac{1}{2}mv^2$. The second term in the energy is related to how much energy is stored in the system at position x due to the force. We call this term the *potential energy*

$$U(x) = -\int_0^x F(x')dx' \tag{3.11}$$

The total energy can then be written as $E = K + U$.

Let's now use the mass on a spring to illustrate this concept. The force on the spring is $F(x) = -kx$ so that the potential energy function is given by

$$U(x) = -\int_0^x (-kx')dx' = \frac{1}{2}kx^2 \tag{3.12}$$

---

[1] The choice of the lower integrant is a bit arbitrary at this point, but rest assured that we will come back to that soon.

and the total energy is

$$E = \frac{1}{2}mv^2 + \frac{1}{2}kx^2 \tag{3.13}$$

Using Newton's equations, we have already solved for the position of the mass as a function of time, and found it to be

$$x(t) = Ae^{i\omega t} + A^* e^{i\omega t} \tag{3.14}$$

where the complex amplitude A depends on the initial position and velocity. Differentiating this equation with respect to time, we can find the velocity

$$v(t) = i\omega Ae^{i\omega t} - i\omega A^* e^{i\omega t} \tag{3.15}$$

Plugging these values into equation 3.13 we find that

$$\frac{1}{2}mv^2 + \frac{1}{2}kx^2 = \frac{1}{2}m\left[i\omega Ae^{i\omega t} - i\omega A^* e^{i\omega t}\right]^2 + \frac{1}{2}k\left[Ae^{i\omega t} + A^* e^{i\omega t}\right]^2 \tag{3.16}$$

$$= \frac{1}{2}m\left[-\omega^2 A^2 e^{2i\omega t} - \omega^2 A^{*2} e^{-2i\omega t} + \omega^2 AA^*\right] \tag{3.17}$$

$$+ \frac{1}{2}k\left[A^2 e^{2i\omega t} + A^{*2} e^{-2i\omega t} + AA^*\right] \tag{3.18}$$

$$= \frac{1}{2}k\left[(A^2 - A^2)e^{2i\omega t} + (A^{*2} - A^{*2})e^{-2i\omega t} + 2|A|^2\right] \tag{3.19}$$

$$= k|A|^2 \tag{3.20}$$

Where we have used the fact that $\omega^2 = k/m$. So, we see that our solution does indeed lead to a constant energy, with value $E = k|A|^2$. You can check for yourself that $|A|^2$ does indeed look like the total energy at time $t = 0$.

One way to look at the different solutions to a set of dynamical equations is to plot them in "phase space." In mathematics and physics, a phase space is a space in which all possible states of a system are represented, with each possible state corresponding to one unique point. For the mechanical systems we've been looking at, phase space consists of all possible values of the position and velocity variables, i.e. a two-dimensional space in which the axes are x and v. Our conservation of energy equation for the harmonic oscillator (Eq. 3.13) can be rewritten as

$$\frac{x^2}{2E/k} + \frac{v^2}{2E/m} = 1 \tag{3.21}$$

This is just the equation for an ellipse in the x–v plane (Fig. 3.1)! Over time, the system repeatedly traces out this ellipse forever. The length of the major and minor axes are governed by the mass, spring stiffness and the total energy. For a given k and m, the size of the ellipse is set by the energy. A system with more energy will move at a larger distance from the origin than a system will less energy. Different initial conditions, i.e. position and velocity, change where on the ellipse the system starts, but not the shape or size of the ellipse.

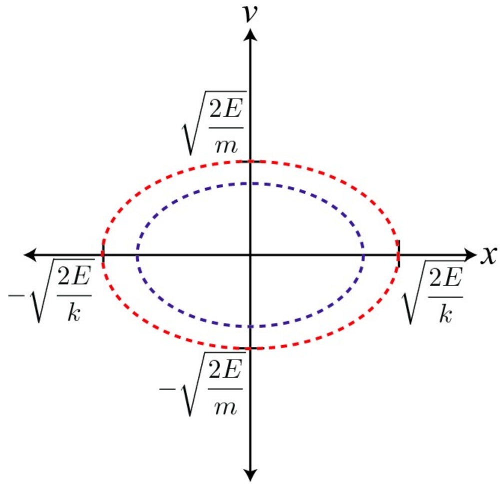


Figure 3.1: Phase space plot of the trajectory of two harmonic oscillators at different energies.

Problem 59: You reach out your dorm room window and throw a ball up into the air. The ball has a mass $m = 0.1\,\mathrm{kg}$, and assume that it leaves your hand when it is at a height $h_0 = 5\,\mathrm{m}$ above the ground. With a little effort you manage to impart an initial (upward) velocity $v_0 = 5\,\mathrm{m/s}$ to the ball. Neglect friction or drag as the ball moves through the air, so the only relevant force is gravity. In case you forget, $g = 9.8\,\mathrm{m/s^2}$.

(a.) What is the initial kinetic energy of the ball (in Joules)?

(b.) Use conservation of energy to determine the maximum height $h_{\max}$ that the ball will reach above the ground.

(c.) As the ball falls back toward the ground, it passes your window again. At the moment when it is exactly at its initial height h_0, what is its velocity? Why? Hint: You don't need a calculator to do this part of the problem.

Problem 60: Consider a simple harmonic oscillator: A mass M and a spring of stiffness κ, with no damping. Assume an initial condition $x(t = 0) = x_0$ and $v(t = 0) = 0$.

(a.) Sketch the potential energy and kinetic energy as a function of time. Label the axes, and relate major features of your sketch to the parameters of the problem.

(b.) What is the value of the potential energy averaged over one cycle of the oscillation?

(c.) What is the value of the kinetic energy averaged over one cycle of the oscillation?

Problem 61: Instead of starting with $F = ma$, one can solve the type of dynamics problems that we have been studying this semester in terms of the conservation of energy.

(a.) For a particle that starts at position x_0 with total energy E at time $t = 0$, show that the position can be found using the following integral

$$t = \int_{x_0}^{x} \frac{\pm dx'}{\sqrt{\frac{2}{m}\left[E - U(x')\right]}} \tag{3.22}$$

What does the ± mean and which sign should you choose?

(b.) Solve for the trajectory $x(t)$ for a harmonic oscillator, $U(x) = \frac{1}{2}kx^2$, using Equation 3.22 for the initial condition: $x(t = 0) = x_0$ and $v(t = 0) = v_0$. Does your answer agree with our previous calculations?

3.2 Conservative forces and potential energy

When we began the semester, we had a little trouble coming up with a definition for a force beyond Newton's second law, i.e. that a force is what causes the acceleration of mass. Now we can go a little farther in that we know that the force can be written as the derivative of the potential energy. Forces of this kind are called *conservative* forces because they, in some sense, conserve mechanical energy.

One important consequence of this is that the work done by a force on an object depends only on the initial and final positions, and is independent of the path taken between these locations. To see this, we can calculate the work done in moving from position x_1 to position x_2 against a force

$$W = \int_{x_1}^{x_2} F(x)dx = -\int_{x_1}^{x_2} \frac{dU(x)}{dx}dx = U(x_1) - U(x_2) \tag{3.23}$$

The final answer only depends on the value of the potential energy at a and b and does not remember how the system moved between these two positions. If you move a mass from height h_1 to height h_2, gravity does work on the mass and the magnitude of this energy doesn't depend on whether you moved the the mass in a straight path between the endpoints or a very convoluted one as in Figure 3.2. Another way of putting this same concept is that no work is done by an external force if an object is moved in a closed path, i.e. it ends up where it started.

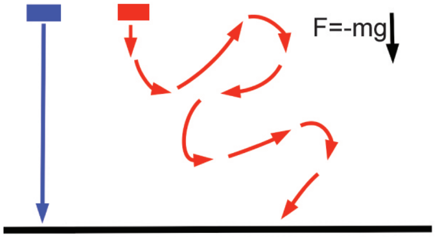


Figure 3.2: Independent of the path taken, the work done by gravity on a block only depends on the starting and ending heights. The potential energy gained by the red and blue blocks is the same, even though the paths are very different.

In our definition of potential energy (Eq. 3.11) we integrated the force from 0 to x. But what is so special about $x = 0$? I could just as easily have chosen a different origin, x_0 from which to calculate the integral

$$U = -\int_{x_0}^{x} F(x')dx' \tag{3.24}$$

These would clearly give different answers for the "amount" of potential energy in the system at position x. It doesn't seem like a good thing that a ball in the air could have 1 Joule of potential energy or a million Joules depending on a choice of origin. Because of this ambiguity, the absolute value of the potential energy is meaningless. However, the *difference* in the potential energy between two states *is* meaningful

$$\begin{aligned}
\Delta U &= U(x_2) - U(x_1) && (3.25)\\
&= -\int_{x_0}^{x_2} F(x')dx' + \int_{x_0}^{x_1} F(x')dx' && (3.26)\\
&= -\left[\int_{x_0}^{x_2} F(x')dx' + \int_{x_1}^{x_0} F(x')dx'\right] && (3.27)\\
&= -\int_{x_1}^{x_2} F(x')dx' && (3.28)
\end{aligned}$$

which doesn't depend on our choice of origin. From now on, when we refer potential energy we will be keeping track of ΔU.

Using these definitions, we found that in an *isolated* system, one in which no *external forces* do work on the system, the total mechanical energy remains constant in time. Changes in the potential energy of the elements in the system are compensated by opposite sign changes in the kinetic energy of the elements.[2]

---

[2] Note that because for conservative forces the change in energy is path independent,

$$\Delta K + \Delta U = 0 \tag{3.29}$$

3.3 Defining the system

We will now look at the effect of an *external* force on a *system*. Imagine that we draw a boundary around the objects that we are interested in, say a mass and a spring, and call everything within the boundary *the system*, and everything outside of the boundary *the environment*. Inside the boundary, the different masses can move around and possess kinetic energy. There can also be elements that generate conservative forces within the system and we will talk about these elements by looking at their potential energies. Outside the boundary, things in the environment can apply forces on the system and transfer energy to/from the system. This transfer of energy will be called "mechanical work", W_{ext}. Our equation for the conservation of energy then equates changes in the energy in the system to the work done by the external environment.

$$\Delta K_{total} + \Delta U_{total} = W_{ext,total} \tag{3.30}$$

In the paragraph above, there is a subtle distinction between the energies in the system, both kinetic and potential, and the external work. Work represents the *transfer* of energy to a system by forces in the environment caused by a change in parameters of the system such as the volume, magnetic or electric fields or the gravitational potential. This transferred energy can then cause an increase or decrease in the energies inside the system. Objects within the system can posses a certain amount of kinetic or potential energy, but an object never "has W Joules of work."

We need to make pick a convention for the sign of the work done by a force. We will define *positive* external work done by the environment on the system as work that *increases* the energy of the system. *Negative* work would then transfer energy out of the system and decrease the system energy[3].

---

we can use the Δ to refer to the total change in a quantity comparing the initial and final states. Unlike the typical trick of using Δ to sneak in calculus with out saying so, we really mean the total change in the kinetic and potential energies and do not need to consider small changes in the limit $\Delta \to 0$.

[3] This choice is arbitrary and we could just as easily reverse all the signs as long as we keep everything consistent.

So, how do we decide what is in the “system” and what is in the “environment”? Well, it actually doesn’t matter in the end. We are free to draw the boundary wherever we want and use Equation 3.30 to calculate the balance of energy. Of course, the conservation of energy must always hold. Lets look at an example to try to make this clear.

Assume you have a mass M suspended from a spring of stiffness k under the influence of gravity. Where do we draw the boundary of the system?

1. It might seem natural to draw the boundary around **mass and the spring**. The spring generates potential energy and gravity is an external force. The change in kinetic energy, i.e. the change in the speed, of the mass plus the change in potential energy from the spring is equal to the external work done by gravity.

   $$\Delta K + \Delta U_{spring} = W_{gravity} \tag{3.31}$$

2. We could, however, draw the boundary around just the **mass**. In this case, there are no force–generating elements inside the boundary and thus no potential energy to consider. So, our equation of conservation of energy becomes

   $$\Delta K = W_{spring} + W_{gravity} \tag{3.32}$$

   Which leads to the same equation for the kinetic energy. The sign of W_{spring} in this case is opposite that of U_{spring} in the previous case because of our definition of the sign of the work. You should work this through in your head to make sure you understand what’s going on.

3. What is so special about the spring? We could equally as well choose the **mass and the earth**(!) as our system. The earth generates potential energy in the system and the spring applies an external force

   $$\Delta K + \Delta U_{gravity} = W_{spring} \tag{3.33}$$

   Again, the same thing.

4. Finally, lets just say that **the whole universe** is the system. The spring and gravity create potential energy and there are no external forces.

   $$\Delta K + \Delta U_{gravity} + \Delta U_{spring} = 0 \tag{3.34}$$

All of these representations are equally as valid and we are free to choose whatever one we want. In practice, one usually tries to choose the definition that makes the solution to a problem easiest, but this is not always apparent at the outset.

Problem 62: (a.) Show that two observers in different frames of reference that are moving relative to each other will measure different positions and velocities, but will agree on the accelerations and forces. Assume that one observer is on a train moving with speed v_0 relative to the ground where a second observer stands

(b.) Because the two observers measure different velocities, they will not agree on the value of the kinetic energy of an object. Show that even though the two observers disagree about this, they do agree that if an external force changes that velocity, then the work done by the force, assuming no potential energy, is given by $W = \Delta K$. It should be reassuring to know that these two observers will measure the same laws of physics even though the numerics may not always agree.

3.4 Internal energy

Before we move on, its worth noting that most objects we encounter in the real world are not "point particles," but instead are rather complicated things. Energy can be stored inside of an object that we can't "see," and therefore our consideration of energy must include these things. In describing the change in energy of a person, an atomistic description in which we describe the position and velocity of every atom and the interactions between them would indeed conform to the type of formalism we've developed previously. But that seems a bit cumbersome, and we'd like to be able to talk about the position of the person and not the 10^{28} atoms that make up him or her. In order to do this, we need to lump all the energy one can store in the interactions between atoms in the body into one quantity, the *internal energy*, E_{int}. Potential energy or external work can, therefore, be converted either into a change in kinetic energy or a change in the internal energy of the object.

$$\Delta K + \Delta U + \Delta E_{int} = W_{ext} \tag{3.35}$$

What types of things can make up an "internal" energy? Anything, really. These include the kinetic motion of molecules within an object[4], a

---

[4] We will soon make a connection between this idea and the temperature of an object

change in the chemical bonding forces between molecules in an object (e.g. by changing the lattice spacing in a crystal), electric and magnetic fields, light ...

Exercise: Come up with three specific examples of an internal energy in a biological organism.

As an example, lets think about how the muscles in your arm work to lift a weight. If you lift the weight slowly from height h_1 to height $h2$, you change the potential energy of the system, which we'll define as you plus the weight, by the amount of work done by the gravitational force

$$\Delta W_{ext} = mg(h_2 - h_1) \tag{3.36}$$

Because you moved the weight slowly, the change in the kinetic energy will be negligible. Furthermore, there aren't any springs or other simple mechanical elements in the system for which a change in potential energy could compensate for the external work. What must be happening is that your body is changing the amount of internal energy stored in your muscles and bones, even though we don't really see it (although we might see some signs of this exertion as you start to turn red and sweat).

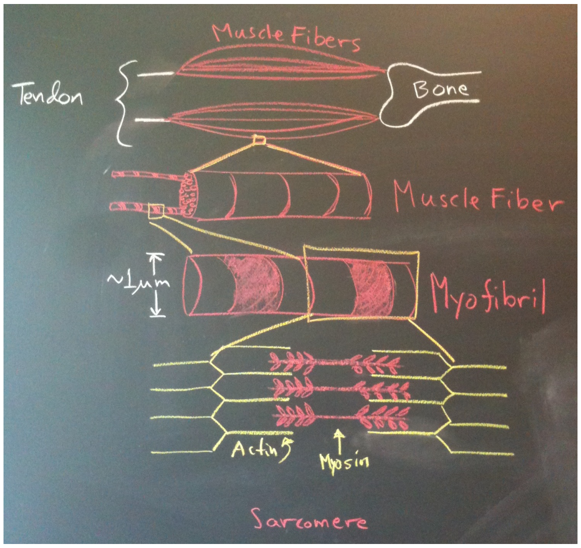


Figure 3.3: The design of a muscle.

The muscles in your body are made up of a series of parallel fibers that can generate mechanical forces by shrinking in length (Fig. 3.3). The shrinking unit within a fiber is called a sarcomere, which is made up of an array of actin filaments (one of the main structural fibers in all of your cells) and a special enzyme called myosin. Myosin is a molecular motor, like the kinesin we saw earlier, that uses *chemical energy* to produce mechanical work. In particular, myosin catalyzes the hydrolysis of ATP: $ATP \rightarrow ADP + Pi$. This process releases some of the energy stored in the ATP molecule and myosin is built such that some of this energy is used to rotate a lever arm within the protein. This rotation slides the myosin "thick" filament relative to the two actin "thin" filaments in the sarcomere so that the unit gets shorter. When you lift a weight, your "internal" energy is changing by an amount $mg(h_2 - h_2)$ and this energy comes from energy stored in the ATP molecules in your muscles.

Problem 63: For every ATP molecule hydrolyzed, myosin slides an actin filament a distance $d \sim 4\,\mathrm{nm}$ along in a sarcomere. The ATP hydrolysis reaction releases $\sim 50\,\mathrm{kJ/mole}$ of energy.

(a.) How much energy is released by *one* ATP molecule?

(b.) If myosin can use all of this energy to do mechanical work, and if it uses one ATP molecule for each step along the actin filament, how much force can it generate while moving through its step of length d?

(c.) How many myosin molecules must be working together when you hold up a 1 kg weight against the force of gravity?

3.5 Mechanical equilibrium

One can deduce many of the properties of a particle's motion by examining the shape of the potential energy function $U(x)$. Because the kinetic energy, $T = \frac{1}{2}mv^2$, is always greater than zero, the total energy E must be greater than or equal to the potential energy for any real–world motion. Let's examine the the potential energy profile sketched in Fig. 3.4. A particle with energy E_4 is unbounded by the potential and is free to move along the x–axis. Of course, it will slow down and speed up due to the potential, but it will not stop or turn around. Now consider a particle with energy E_3 moving to the left towards x_7. The particle will keep moving, speeding up and slowing down, until it reaches x_7, where the potential energy is equal to the total energy. At this point the kinetic energy must be zero and the particle stops. Because of the slope of $U(x)$ at that point, the particle will feel a force in the $+x$–direction. It will then begin to move and continue off to infinity. A particle with energy E_1 is bounded in the potential well and oscillates between x_1 and x_2 forever. If the particle instead has energy E_2 it can exist in one of two different wells, oscillating between x_3 and x_4 or between x_5 and x_6. Because the energy barrier between the wells is greater than E_2, the particle stays in only one well forever.

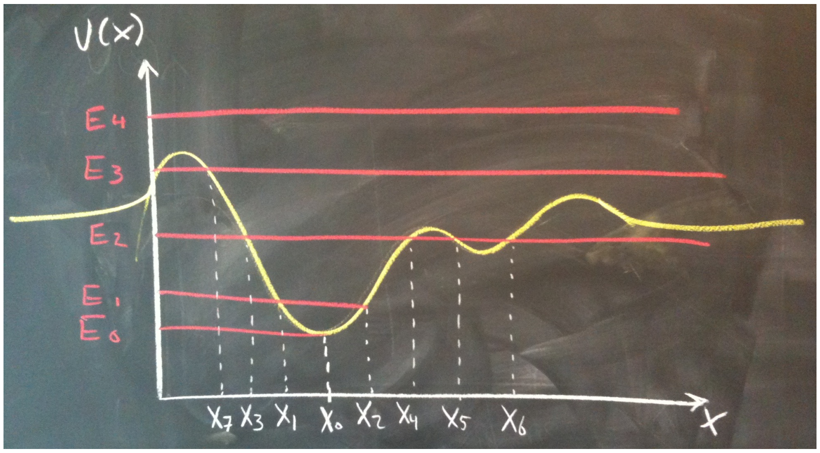


Figure 3.4:

If the particle has energy E_0 there is only one position where it can lie, at x_0, where it remains at rest with $E = U$. Newton's laws tell us that if the net force on a object is zero, then the acceleration of that object is zero and this state we call *mechanical equilibrium.* Mathematically, if an object experiences a set of forces $\{F_i\}$, then at equilibrium we can write

$$\sum_i F_i(x) = 0 \tag{3.37}$$

If these are conservative forces, then we can write $F_i(x) = -\frac{\partial U_i(x)}{\partial x}$. At equilibrium we have

$$-\sum_i \frac{\partial U_i(x)}{\partial x} = 0 \tag{3.38}$$

Taking the derivative out of the sum, we find

$$\frac{\partial}{\partial x}\sum_i U_i(x) = \frac{\partial U_{total}(x)}{\partial x} = 0 \tag{3.39}$$

Since the derivative of the total potential energy with respect to x is zero, the potential energy must be an extremum (a minimum, maximum or inflection point) at equilibrium. An equilibrium point can be stable or unstable to perturbations depending on the sign of the second derivative of the potential energy. If we look at the force on an object a distance δx from an equilibrium point we find

$$F(x_{eq}+\delta x) = -\left.\frac{\partial U(x)}{\partial x}\right|_{x=x_{eq}+\delta x} \tag{3.40}$$

$$\approx -\frac{\partial U(x_{eq})}{\partial x} - \frac{\partial^2 U(x_{eq})}{\partial x^2}\delta x \tag{3.41}$$

$$= -\frac{\partial^2 U(x_{eq})}{\partial x^2}\delta x \tag{3.42}$$

This looks like a spring with a restoring force that pulls the object towards the equilibrium point if $\frac{\partial^2 U(x_{eq})}{\partial x^2} > 0$, i.e. if the potential energy is a minimum at the equilibrium point. This is called a *stable* equilibrium point. If $\frac{\partial^2 U(x_{eq})}{\partial x^2} < 0$ and the equilibrium point is a maximum then the force pushes the object farther away from x_{eq} and the point is an *unstable* equilibrium point.

As an example, lets consider a mass m attached to the end of a spring of stiffness k under the influence of gravity. The total potential energy is given by

$$U(x) = \frac{1}{2}k(x-x_0)^2 - mg(x-x_0) \tag{3.43}$$

To find the equilibrium point(s), we take the derivative and set it to zero

$$\frac{dU}{dx} = k(x_{eq}-x_0) - mg = 0 \tag{3.44}$$

Which gives $x_{eq} = x_0 + \frac{mg}{k}$. The second derivative of the potential energy at x_{eq} is just k which is greater than zero so that the energy is a minimum at the equilibrium point at it is stable as you could have guesses.

Problem 64: Consider a particle under the influence of a force

$$F(x) = -kx + \frac{k}{\beta}x^3 \tag{3.45}$$

where k and β are both positive constants.

(a.) Solve for the potential energy $U(x)$.
(b.) Describe the motion for particles with different energies at various positions.
(c.) What happens when $E = \frac{1}{4}k\beta$?

3.6 Nonconservative forces: Friction and other ways to lose energy

Your intuition should be telling you that there is something about these idealized pictures that doesn't quite match with your experience. First of all, towards the beginning of the class we learned about friction and wind resistance, forces whose magnitudes are proportional not to position, but to velocity and the velocity squared respectively. For these types of forces, a potential of the form $U(x)$ clearly makes no sense. Its not the position that governs the force but how fast the position is changing. The work done by these forces depends not on the endpoints, but on the speed an object moves along a particular path between the endpoints. We will call these types of forces *nonconservative*.[5] For these types of forces, you can not define a potential energy and the equation for the conservation of energy we derived before doesn't hold! So, what good is a conservation law if it only works for some kinds of forces? Soon, we'll amend our definitions to patch this up, but for now lets put the conservation of energy on hold.

As an example, consider an object moving with a constant velocity in the presence of a friction force

$$F(x) = -\gamma \dot{x} \tag{3.46}$$

If the object travels a distance $\Delta x = v\Delta t$, then the work done by the force on the object is

$$W = F(x)\Delta x = -\gamma v \Delta x = -\gamma v\,(v\Delta t) = -\gamma v^2 \Delta t \tag{3.47}$$

The work does not depend on the position (we could repeat the experiment 2 meters to the right and nothing would change), or even the direction, but

---

[5] The idea of nonconservative forces is somewhat misleading and is usually due to the macroscopic treatment of something that is really the sum of many microscopic parts. For example, friction is caused by the conservative forces between the atoms in a moving object and the thing its moving against. Each one of these microscopic forces is conservative and can be written as the gradient of a potential. But, the resultant force on the object as a whole appears to be nonconservative. In reality, there are no nonconservative forces in the universe in that we know of.

instead on the amount of time the object spent moving. If the object moves in a closed path, say out a meter and back, the object looses energy the whole time even though it started and stopped at the exact same position.

Problem 65: Energy of an underdamped oscillator

(a.) Derive an expression for the energy of an underdamped oscillator as treated in Chapter 2.3.

(b.) Graph the energy as a function of time.

(c.) Make a phase-space plot of the trajectory of the underdamped oscillator. Does the system move in a closed orbit?

Problem 66: Derive the formula for the energy of a spring–mass system in which the drag force is equal to $F_{drag} = -\epsilon \frac{dx}{dt}^2$ which is the correct form for air resistance.

Problem 67: Imagine that we drop a ball of mass m from an initial height h_0.

(a.) Neglecting friction, use conservation of energy to plot the ball's velocity $v(t) = dh/dt$ as a function of its height $h(t)$.

(b.) Suppose that as the ball falls through the air it experiences a drag force $-\gamma(dh/dt)$; again it starts from a height h_0. Without solving any differential equations, show how the plot of $v(t)$ vs. $h(t)$ will change as a result of this friction.

(c.) Solve the differential equation corresponding to $F = ma$ to find an expression for $h(t)$ in the presence of friction. Show that there are simple limiting behaviors for small t and large t. Plot $h(t)$ and indicate these simple limits, as well as the time scale on which the plot crosses over from one limit to the other.

(d.) Plot the amount of time T required to hit the ground $[h(T) = 0]$ as a function of the initial height h_0. Hint: The small t and large t limits in [c] correspond to small h_0 and large h_0 regions of this plot.

So, we've seen that friction forces can't be described by a potential and the conservation laws we wrote before don't seem to hold. Is friction the only example where this breaks down? Lets return to the weight lifting example. After you've lifted the weight, what if you try to hold it up forever with your muscles. From experience, we know that you'll get tired, but why? The position of the weight isn't changing, so there's no change in gravitational potential energy. Nothing is moving, so there's no friction or kinetic energy. Why is it that your body has to keep using up energy to hold the weight up? It turns out that your muscles have no way to "lock in" a position. Instead, they have to keep burning ATP to maintain a certain degree of muscle fiber shrinkage, which is why you get tired. But where does all this energy go?

3.7 Gaining all the energy back: The first law of Thermodynamics

So far, we have only talked about one method of transferring energy into or out of a system – through mechanical work. There is a second way of transferring energy, and that is through heat. We'll clarify what heat is in detail when we tackle the subject of Thermodynamics later in the term, but it should comfort you that there is a connection between heat and ways of losing energy like friction.

If you take the heat into account, and we write down all of the energy (including the energy in the system and the work done and heat transferred) then energy *really is* conserved. This is known as the first law of thermodynamics. Towards the end of the course we will see that the conservation of energy is implied by a very deep principle, that the laws of Nature are the same over time, i.e. that if you do an experiment today you will get the same answer if you repeat the experiment tomorrow. By taking this concept seriously, one can show that the conservation of energy must hold!

Stated another way, the first law says that **the energy in the universe is always conserved**. No matter how we look at it, there are no ways of creating or destroying energy, just ways of moving it around. This leads us to a nice conclusion, that there is really only one universe – or at least the conclusion that our universe can not exchange energy with any other universes.[6]

[Need to integrate these problems into previous sections, check for redundancy.]

Problem 68: You reach out your dorm room window and throw a ball up into the air. The ball has a mass $m = 0.1\,\mathrm{kg}$, and assume that it leaves your hand when it is at a height $h_0 = 5\,\mathrm{m}$ above the ground. With a little effort you manage to impart an initial (upward) velocity $v_0 = 5\,\mathrm{m/s}$ to the ball. Neglect friction or drag as the ball moves through the air, so the only relevant force is gravity. In case you forget, $g = 9.8\,\mathrm{m/s^2}$.

(a.) What is the initial kinetic energy of the ball (in Joules)?

(b.) Use conservation of energy to determine the maximum height $h_{\max}$ that the ball will reach above the ground.

---

[6] At this point the discussion becomes a bit philosophical. What does it mean to have another universe in which you can't exchange energy and hence can't see or probe in any meaningful way? We'll leave that discussion for another class (perhaps in another department).

(c.) As the ball falls back toward the ground, it passes your window again. At the moment when it is exactly at its initial height h_0, what is its velocity? Why? Hint: You don't need a calculator to do this part of the problem.

Problem 69: Imagine that we drop a ball of mass m from an initial height h_0.

(a.) Neglecting friction, use conservation of energy to plot the ball's velocity $v(t) = dh/dt$ as a function of its height $h(t)$.

(b.) Suppose that as the ball falls through the air it experiences a drag force $-\gamma(dh/dt)$; again is starts from a height h_0. Without solving any differential equations, show how the plot of $v(t)$ vs. $h(t)$ will change as a result of this friction.

(c.) Solve the differential equation corresponding to $F = ma$ to find an expression for $h(t)$ in the presence of friction. Show that there are simple limiting behaviors for small t and large t. Plot $h(t)$ and indicate these simple limits, as well as the time scale on which the plot crosses over from one limit to the other.

(d.) Plot the amount of time T required to hit the ground $[h(T) = 0]$ as a function of the initial height h_0. Hint: The small t and large t limits in [c] correspond to small h_0 and large h_0 regions of this plot.

Problem 70: Consider a simple harmonic oscillator: A mass M and a spring of stiffness κ, with no damping. Assume an initial condition $x(t = 0) = x_0$ and $v(t = 0) = 0$.

(a.) Sketch the potential energy and kinetic energy as a function of time. Label the axes, and relate major features of your sketch to the parameters of the problem.

(b.) What is the value of the potential energy averaged over one cycle of the oscillation?

(c.) What is the value of the kinetic energy averaged over one cycle of the oscillation?

Problem 71: Inside your muscle there are "motor molecules" called myosin that convert the chemical energy of ATP into mechanical work. As they do this, the myosin molecules move in steps of size $d \sim 4\,\text{nm}$ along filaments of actin. Breaking down the ATP molecule releases $\sim 50\,\text{kJ/mole}$ of energy.

(a.) How much energy is released by *one* ATP molecule?

(b.) If myosin can use all of this energy to do mechanical work, and if it uses one ATP molecule for each step along the actin filament, how much force can it generate while moving through its step of length d?

(c.) How many myosin molecules must be working together when you hold up a 1 kg weight against the force of gravity?

Problem 72: Consider a particle of mass m that moves in one dimension x. In the absence of damping, Newton's equation ($F = ma$) can be written as

$$m\frac{d^2x}{dt^2} = -\frac{dV(x)}{dx}, \tag{3.48}$$

where $V(x)$ is the potential energy. Conservation of energy is the statement that $dE/dt = 0$, where

$$E = \frac{1}{2}m\left(\frac{dx}{dt}\right)^2 + V(x). \tag{3.49}$$

If we add damping to the system, Newton's equation becomes

$$m\frac{d^2x}{dt^2} = -\gamma\frac{dx}{dt} - \frac{dV(x)}{dx}. \tag{3.50}$$

Show that if $x(t)$ follows Eq (3.50), then the energy E decreases in time as $\frac{dE}{dt} = -\gamma v^2$. Note that this corresponds to your intuition—viscous drag "sucks energy" out of the motion. Hint: Remember the chain rule,

$$\frac{d}{dt}g(x) = \frac{dg(x)}{dx} \cdot \frac{dx(t)}{dt}. \tag{3.51}$$

Chapter 4

We are not the center of the universe

4.1 Conservation of $\tilde{\mathbf{P}}$ and $\tilde{\mathbf{L}}$

We have discussed the conservation of energy, showing how the existence of a potential energy constrains the possible form of forces that enter Netwon's $F = ma$. In these lectures we'll discuss the conservation of momentum and angular momentum. We will start with a fairly conventional freshman physics point of view, namely that conservation of momentum follows from the law of action and reaction. Then we will see that there is a deeper view, namely that conservation of momentum follows from insisting that our description of the world in terms of a potential energy as a function of position(s) doesn't depend on where we choose to put the origin of coordinate system. This independence is called "invariance" to translations, and the idea that conservation laws follow from invariance principles is one of the fundamental ideas of modern physics. After the discussion of momentum we will turn to angular momentum, which introduces some complications but exposes the same link between invariance and conservation. As we shall see, invariance is the statement that our description of the world, in a coordinate system that we chose, should be the same as that obtained by a different person who might choose a different coordinate system. In this sense there is no special coordinate system in which one obtains uniquely correct answers. This seems simple enough, but it means that our personal, human point of view is not privileged.

Consider a system of particles in which the different particles apply forces to one another in pairs. Then when we write $F = ma$ for the i^{th} particle,

$$\begin{aligned} m_\mathrm{i}\vec{a}_\mathrm{i} \equiv \frac{d\vec{p}_\mathrm{i}}{dt} &= \vec{F}_\mathrm{i} && (4.1)\\ &= \sum_\mathrm{j} \vec{F}_{\mathrm{j}\to\mathrm{i}}, && (4.2)\end{aligned}$$

where $\vec{p}_\mathrm{i} \equiv m_\mathrm{i}\vec{v}_\mathrm{i}$ is the *momentum* of the i^{th} particle, and$\vec{F}_{\mathrm{j}\to\mathrm{i}}$ is the force which particle j exerts on particle i. The law of action and reaction is then the statement that

$$\vec{F}_{\mathrm{j}\to\mathrm{i}} = -\vec{F}_{\mathrm{i}\to\mathrm{j}}. \tag{4.3}$$

This is enough to show that the total momentum

$$\vec{P}_\mathrm{total} = \sum_\mathrm{i} \vec{p}_\mathrm{i} \tag{4.4}$$

is conserved. To show this we just compute the time derivative of $\vec{P}$ by substitution:

$$\begin{aligned} \frac{d\vec{P}_\mathrm{total}}{dt} &= \sum_\mathrm{i} \frac{d\vec{p}_\mathrm{i}}{dt} && (4.5)\\ &= \sum_\mathrm{i} \vec{F}_\mathrm{i} && (4.6)\\ &= \sum_\mathrm{i}\sum_\mathrm{j} \vec{F}_{\mathrm{j}\to\mathrm{i}} && (4.7)\\ &= \sum_{\mathrm{all\ pairs\ ij}} \vec{F}_{\mathrm{j}\to\mathrm{i}} && (4.8)\end{aligned}$$

But when we sum over all pairs, we must count (for example) the pair (1,7) and the pair (7,1). Thus the sum over all pairs includes both the term $\vec{F}_{1\to 7}$ and the term $\vec{F}_{7\to 1}$. But when we add these two terms we get zero, because of Eq. (4.3), and this is true for every pair ij. Thus

$$\sum_{\mathrm{all\ pairs\ ij}} \vec{F}_{\mathrm{j}\to\mathrm{i}} = 0, \tag{4.9}$$

and hence

$$\frac{d\vec{P}_\mathrm{total}}{dt} = 0, \tag{4.10}$$

which means that momentum is conserved.

There is a different way to go at proving conservation of momentum, and this illustrates the general connection between conservation laws and symmetries or invariances. We know that forces can be found by taking derivatives of the potential energy. The potential energy is a function of the (vector) positions of all the particles:

$$V = V(\vec{r}_1, \vec{r}_2, \cdots, \vec{r}_{\mathrm{N}}), \tag{4.11}$$

where there are N particles in our system. It sounds reasonable that, if the potential energy is going to mean something, it should not depend on the coordinate system we use to define the locations of all the particles. In particular, if we take our coordinate system with us as we move one step, all of the position vectors $\vec{r}_{\mathrm{i}}$ will shift by a constant amount. To make things simple, let's focus on shifts along the x axis. Then it is useful to explicit about the components of the vector positions: $\vec{r}_{\mathrm{i}} \equiv (x_{\mathrm{i}}, y_{\mathrm{i}}, z_{\mathrm{i}})$. We can write the potential energy as

$$V = V(x_1, x_2, \cdots, x_{\mathrm{N}}; y_1, y_2, \cdots, y_{\mathrm{N}}; z_1, z_2, \cdots, z_{\mathrm{N}}), \tag{4.12}$$

and then if we shift our coordinate system by an distance d along the x axis the potential energy becomes

$$V \to V(x_1 + d, x_2 + d, \cdots, x_{\mathrm{N}} + d; y_1, y_2, \cdots, y_{\mathrm{N}}; z_1, z_2, \cdots, z_{\mathrm{N}}). \tag{4.13}$$

What we would like is that this transformation actually leaves the potential energy *unchanged*, so that

$$\begin{aligned} &V(x_1, x_2, \cdots, x_{\mathrm{N}}; y_1, y_2, \cdots, y_{\mathrm{N}}; z_1, z_2, \cdots, z_{\mathrm{N}}) \\ &\qquad = V(x_1 + d, x_2 + d, \cdots, x_{\mathrm{N}} + d; y_1, y_2, \cdots, y_{\mathrm{N}}; z_1, z_2, \cdots, z_{\mathrm{N}}). \end{aligned} \tag{4.14}$$

Obviously not all the potential functions that we might write down have this property, so our possible models of the world are constrained by this invariance.

We'd like Eq (4.14) to a be global statement, valid for any value of $\vec{d}$. But as is often true in calculus, we can check for global constancy by considering only small shifts: the global statement that something is constant is the local statement that derivatives are zero, applied at every point. Thus we look at very small d, so we can use a Taylor series expansion. In doing this, it's important to remember here that we can do an expansion for x_1

while holding all the other $x_{\rm i}$ fixed, so that there really isn't anything special about our use of partial derivatives here! So, we have

$$\begin{aligned} &V(x_1+d, x_2+d, \cdots, x_{\rm N}+d; y_1, y_2, \cdots, y_{\rm N}; z_1, z_2, \cdots, z_{\rm N}) \\ &\quad \approx V(x_1, x_2, \cdots, x_{\rm N}; y_1, y_2, \cdots, y_{\rm N}; z_1, z_2, \cdots, z_{\rm N}) \\ &\qquad + \left[d\frac{\partial V}{\partial x_1} + d\frac{\partial V}{\partial x_2} + \cdots + d\frac{\partial V}{\partial x_N} \right] \end{aligned} \tag{4.15}$$

Then to make sure that V doesn't change, we must have

$$d\frac{\partial V}{\partial x_1} + d\frac{\partial V}{\partial x_2} + \cdots + d\frac{\partial V}{\partial x_N} = 0. \tag{4.16}$$

Notice that we can take out the common factor of d, so really this is

$$\frac{\partial V}{\partial x_1} + \frac{\partial V}{\partial x_2} + \cdots + \frac{\partial V}{\partial x_N} = 0. \tag{4.17}$$

But $-\partial V/\partial x_{\rm i}$ is just the force acting on particle i (in the x direction). So we have just shown that the sum of all the forces must be zero, independent of any assumptions about forces acting in paris or ideas about action and reaction: The result follows from the invariance of the potential energy with respect to translations of our coordinate system. Notice that we did this specifically for the x direction, but we could equally have looked along y or z, and hence we know that the sum of the vector forces also is zero.

To finish this discussion, let's be clear once more that the zero sum of all forces results in conservation of momentum. To keep things simple let's just focus on the x components:

$$m_{\rm i}\frac{d^2x_{\rm i}}{dt^2} \equiv \frac{dp^x_{\rm i}}{dt} = -\frac{\partial V}{\partial x_{\rm i}} \tag{4.18}$$

$$\Rightarrow \sum_{\rm i=1}^{N} \frac{dp^x_{\rm i}}{dt} = -\sum_{\rm i=1}^{N} \frac{\partial V}{\partial x_{\rm i}} \tag{4.19}$$

$$\frac{d}{dt}\left[\sum_{\rm i=1}^{N} p^x_{\rm i}\right] = -\sum_{\rm i=1}^{N} \frac{\partial V}{\partial x_{\rm i}} \tag{4.20}$$

$$= 0, \tag{4.21}$$

where in the last step we use Eq (4.17). So what we have shown is that the x component of the total momentum does not change with time. Again we could have done this for the y or z components, and so really we know that *demanding that the potential energy be unchanged under translations implies conservation of momentum.*

It is good to think a bit about this result, which really is quite remarkable. When we say that we want our description of the world to be the same no matter what we choose for the origin of our coordinate system, this sounds like a philosophical statement: we want our mathematical models to have certain "nice" properties. But this particular nice property implies the conservation of momentum, and this a statement about measurable quantities in the physical world around us!

Let's keep going with the idea of invariance under changes of coordinate system. In addition to invariance under translations, we'd also like to insist on invariance under rotations—it shouldn't matter which way we are looking when we decide to set up our coordinate system, just as it doesn't matter where we are standing. Suppose we start with some coordinate system in which the particles are at positions $\vec{r}_1, \vec{r}_2, \cdots, \vec{r}_{\rm N}$. Now we turn by some angle θ, and these positions become $\vec{r}\,'_1, \vec{r}\,'_2, \cdots, \vec{r}\,'_{\rm N}$ in our new coordinate system. We want to insist that

$$V(\vec{r}_1, \vec{r}_2, \cdots, \vec{r}_{\rm N}) = V(\vec{r}\,'_1, \vec{r}\,'_2, \cdots, \vec{r}\,'_{\rm N}). \tag{4.22}$$

Obviously in order to impose this condition we have to understand how the positions $\vec{r}_{\rm i}$ tranform into $\vec{r}\,'_{\rm i}$ when we rotate.

For simplicity let's work in two dimensional space. Then by the vector position of $\vec{r}_{\rm i}$ the i$^{\rm th}$ particle what we really mean is the pair $x_{\rm i}, y_{\rm i}$:

$$\vec{r}_{\rm i} = x_{\rm i}\hat{\mathbf{x}} + y_{\rm i}\hat{\mathbf{y}}, \tag{4.23}$$

where $\hat{\mathbf{x}}$ and $\hat{\mathbf{y}}$ are unit vectors in the x and y directions, respectively (also called $\hat{\mathbf{i}}$ and $\hat{\mathbf{j}}$). Now if we rotate our x and y coordinate system through an angle θ, then the coordinates of a particle will transform as

$$x_{\rm i} \to x'_{\rm i} = x_{\rm i}\cos\theta + y_{\rm i}\sin\theta \tag{4.24}$$

$$y_{\rm i} \to y'_{\rm i} = y_{\rm i}\cos\theta - x_{\rm i}\sin\theta \tag{4.25}$$

It will turn out that we want to know what happens when we make a *small* turn, so that θ is very small. In fact so small that we only want to keep terms linear in θ. Why? Because (as in the discussion of momentum conservation, where we took $\vec{d}$ to be small) we are going to impose our condition on the potential energy by insisting that the derivative of the potential energy with respect to the rotation angle θ is zero, since this is enough to make sure that V never changes no matter how much we rotate.

With this in mind, let's recall that for small θ,

$$\cos\theta \approx 1 - \frac{1}{2}\theta^2 + \cdots, \tag{4.26}$$

$$\sin\theta \approx \theta - \frac{1}{3!}\theta^3 + \cdots, \tag{4.27}$$

so if we want to keep linear terms in θ, we approximate $\cos\theta$ as being 1, and $\sin\theta$ as being θ:

$$
\begin{aligned}
x_{\mathrm{i}} \to x'_{\mathrm{i}} &= x_{\mathrm{i}} + \theta y_{\mathrm{i}} && (4.28)\\
y_{\mathrm{i}} \to y'_{\mathrm{i}} &= y_{\mathrm{i}} - \theta x_{\mathrm{i}}. && (4.29)
\end{aligned}
$$

So, what happens to the potential energy under this transformation?

We start with

$$V(\vec{r}_1, \vec{r}_2, \cdots) = V(x_1, y_1, x_2, y_2, \cdots) \tag{4.30}$$

because we agree to work in two dimensions (you can do all of this in 3D but the algebra is more complicated!). Thus when we rotate our coordinate system by a small angle θ the potential transforms as

$$V(x_1, y_1, x_2, y_2, \cdots) \to V(x_1+\theta y_1, y_1-\theta x_1, x_2+\theta y_2, y_2-\theta x_2, \cdots); \tag{4.31}$$

remember that $\cdots$ means that we keep going until we have listed the coordinates of all N particles in the system.

Since θ is small we can use the Taylor series idea once more:

$$
\begin{aligned}
&V(x_1 + \theta y_1, y_1 - \theta x_1, x_2 + \theta y_2, y_2 - \theta x_2, \cdots)\\
&\quad\approx V(\vec{x}_1, \vec{x}_2, \cdots) + \theta y_1 \frac{\partial V}{\partial x_1} - \theta x_1 \frac{\partial V}{\partial y_1} + \theta y_2 \frac{\partial V}{\partial x_2} - \theta x_2 \frac{\partial V}{\partial y_2} + \cdots .
\end{aligned}
\tag{4.32}
$$

Collecting all of the terms, we find the transformation of V under small rotations:

$$V \to V - \theta \sum_{\mathrm{i}=1}^{\mathrm{N}} \left(x_{\mathrm{i}} \frac{\partial V}{\partial y_{\mathrm{i}}} - y_{\mathrm{i}} \frac{\partial V}{\partial x_{\mathrm{i}}} \right). \tag{4.33}$$

Now what appears under the summation in Eq. (4.33) is an interesting combination of things. First, remember that forces are related to the derivatives of the potential energy:

$$\vec{F}_{\mathrm{i}} = \left(-\frac{\partial V}{\partial x_{\mathrm{i}}} \right) \hat{\mathbf{x}} + \left(-\frac{\partial V}{\partial y_{\mathrm{i}}} \right) \hat{\mathbf{y}}. \tag{4.34}$$

The second thing to remember is about cross products. If we have two vectors in two dimensional (xy) space,

$$
\begin{aligned}
\vec{a} &= a_x \hat{\mathbf{x}} + a_y \hat{\mathbf{y}} && (4.35)\\
\vec{b} &= b_x \hat{\mathbf{x}} + b_y \hat{\mathbf{y}}, && (4.36)
\end{aligned}
$$

then their cross product $\vec{a}\times\vec{b}$ is a vector pointing out of the xy plane in the z direction,

$$\vec{a}\times\vec{b} = (a_x b_y - a_y b_x)\hat{\mathbf{z}}. \tag{4.37}$$

Third, recall that $\vec{r}_{\rm i} = x_i\hat{\mathbf{x}}+y_{\rm i}\hat{\mathbf{y}}$. Now we can put these three things together to realize that

$$x_{\rm i}\frac{\partial V}{\partial y_{\rm i}} - y_{\rm i}\frac{\partial V}{\partial x_{\rm i}} = -\hat{\mathbf{z}}\cdot(\vec{r}_{\rm i}\times\vec{F}_{\rm i}). \tag{4.38}$$

[Be sure to check that you understand these steps!]

The object $\vec{\tau}_{\rm i} = \vec{r}_{\rm i}\times\vec{F}_{\rm i}$ is something you have seen in your high school physics courses: it is the torque on the i^{th} particle. Notice that the torque always points in the $\hat{\mathbf{z}}$ direction if our particles are confined to the xy plane, which is why sometimes we forget that torque is a vector. So it's interesting that when we ask how the potential energy transforms under rotations, the torque just pops out:

$$V \to V + \theta\hat{\mathbf{z}}\cdot\left(\sum_{\rm i=1}^{\rm N}\vec{\tau}_{\rm i}\right). \tag{4.39}$$

Furthermore, if we want to have *invariance* under rotations then the coefficient of θ needs to be zero, so we must have

$$\sum_{\rm i=1}^{\rm N}\vec{\tau}_{\rm i} = 0. \tag{4.40}$$

But now we are almost done. Let's look at Netwon's equations,

$$\frac{d\vec{p}_{\rm i}}{dt} = \vec{F}_{\rm i}. \tag{4.41}$$

Notice that we have one of these (vector) equations for each particle. Since we know something about torques, it makes sense to take the cross product of each side of the equation with the vector $\vec{r}_{\rm i}$:

$$\vec{r}_{\rm i}\times\frac{d\vec{p}_{\rm i}}{dt} = \vec{r}_{\rm i}\times\vec{F}_{\rm i} = \vec{\tau}_{\rm i}. \tag{4.42}$$

The combination on the left of this equation is a little awkward, so we can make it nicer by realizing that

$$\frac{d(\vec{r}_{\rm i}\times\vec{p}_{\rm i})}{dt} = \frac{d\vec{r}_{\rm i}}{dt}\times\vec{p}_{\rm i} + \vec{r}_{\rm i}\times\frac{d\vec{p}_{\rm i}}{dt}. \tag{4.43}$$

Since $\vec{p}_{\rm i} = m_{\rm i}(d\vec{r}_{\rm i}/dt)$, the term

$$\frac{d\vec{r}_{\rm i}}{dt}\times\vec{p}_{\rm i} = m_{\rm i}\frac{d\vec{r}_{\rm i}}{dt}\times\frac{d\vec{r}_{\rm i}}{dt} = 0, \tag{4.44}$$

since the cross product of a vector with itself is zero. Thus

$$\vec{r}_{\rm i}\times\frac{d\vec{p}_{\rm i}}{dt} = \frac{d(\vec{r}_{\rm i}\times\vec{p}_{\rm i})}{dt}, \tag{4.45}$$

and hence Newton's equations imply that

$$\frac{d(\vec{r}_{\rm i}\times\vec{p}_{\rm i})}{dt} = \vec{\tau}_{\rm i}. \tag{4.46}$$

As you know, we call the combination

$$\vec{L}_{\rm i} \equiv \vec{r}_{\rm i}\times\vec{p}_{\rm i} \tag{4.47}$$

the angular momentum of the $\rm i^{th}$ particle; Eq. (4.46) usually is written as

$$\frac{d\vec{L}_{\rm i}}{dt} = \vec{\tau}_{\rm i}. \tag{4.48}$$

Finally, let's add up all these equations (one for each particle):

$$\sum_{\rm i=1}^{\rm N}\frac{d\vec{L}_{\rm i}}{dt} = \sum_{\rm i=1}^{\rm N}\vec{\tau}_{\rm i} \tag{4.49}$$

$$\frac{d\vec{L}_{\rm total}}{dt} = \sum_{\rm i=1}^{\rm N}\vec{\tau}_{\rm i}, \tag{4.50}$$

where the total angular momentum is the sum of individual angular momenta, by analogy with the total (linear) momentum $\vec{P}$ defined above,

$$\vec{L}_{\rm total} = \sum_{\rm i=1}^{\rm N}\vec{L}_{\rm i}. \tag{4.51}$$

Now put Eq. (4.50) together with Eq. (4.40), and we find

$$\frac{d\vec{L}_{\rm total}}{dt} = 0, \tag{4.52}$$

which means that angular momentum is conserved.

To recap:

- The equation

  $$\frac{d\vec{L}_{\rm i}}{dt} = \vec{\tau}_{\rm i} \tag{4.53}$$

  is just $F = ma$ in disguise (for particle i), so there is nothing really new here.

- In principle the forces $\vec{F}_{\rm i}$ can be arbitrary functions of position.

- If we assume that

  a. forces are derived from a potential energy V,
  b. the potential energy does not depend on the coordinate system is which we measure the particle positions, and
  c. in particular V is invariant under rotations of our coordinate system,

  then the total angular momentum $\vec{L}_{\rm total} = \sum \vec{L}_{\rm i}$ is conserved,

  $$\frac{d\vec{L}_{\rm total}}{dt} = 0. \tag{4.54}$$

4.2 Universality of gravitation

[This section remains to be written. Current students should check on `blackboard` to see if some more informal notes are posted.]

4.3 Kepler's laws

You are familiar with the idea that one can solve some mechanics problems using only conservation of energy and (linear) momentum. Thus, some of what we see as objects move around in the world is a direct consequence of these conservation laws rather than being the result of some detailed "mechanism." It is nice to give an example of how conservation of angular momentum has similarly powerful (and perhaps more famous) consquences.

We recall that roughly 500 years ago, Kepler made one of the great breakthroughs (not just in physics, but in human thought), providing evidence that planet motions as describe by Tycho Brahe are much more simply described in a world model with the sun (rather than the earth) at the center. I don't think we can overstate the importance of realizing that we are not at the center of the universe.

Quantitatively, Kepler noticed several things (Kepler's laws): The orbits of planets around the sun are elliptical, the periods of the orbits are related to their radii, and as the orbit proceeds it sweeps out equal area in equal times. Of these, the equal area law is the one which is related to conservation of angular momentum.

If the orbits were circular it would be trivial that they sweep out area at a constant rate. The equal area law is, in a sense, all that is left of the 'perfection' that people had sought with circular orbits.

If we are at a distance r from the center of our coordinate system (the sun), and we move by an angle $\Delta\theta$, then for small angles the area that is swept out is

$$\Delta A = \frac{1}{2} r^2 \Delta\theta = \left(\frac{1}{2} r^2 \frac{d\theta}{dt}\right) \Delta t. \tag{4.55}$$

The equal area law is the statement that the term in parentheses,

$$\frac{dA}{dt} = \frac{1}{2} r^2 \frac{d\theta}{dt}, \tag{4.56}$$

is a constant, independent of time.

We know that angular momentum is conserved, so let's see if this has something to do with the equal area law. The vector position of the planet can always be written as $\vec{r} = r\hat{\mathbf{r}}$, where $\hat{\mathbf{r}}$ is a unit vector pointing outward toward the current location. The velocity consists of components in the $\hat{\mathbf{r}}$ direction and in the $\hat{\theta}$ direction, around the curve,

$$\frac{d\vec{r}}{dt} = \frac{dr}{dt}\hat{\mathbf{r}} + r\frac{d\theta}{dt}\hat{\theta}. \tag{4.57}$$

Hence

$$\begin{aligned} \vec{p} \equiv m\frac{d\vec{r}}{dt} &= m\frac{dr}{dt}\hat{\mathbf{r}} + mr\frac{d\theta}{dt}\hat{\theta} && (4.58) \\ \vec{L} \equiv \vec{r}\times\vec{p} &= (r\hat{\mathbf{r}})\times\left(m\frac{dr}{dt}\hat{\mathbf{r}}\right) + (r\hat{\mathbf{r}})\times\left(mr\frac{d\theta}{dt}\hat{\theta}\right). && (4.59) \end{aligned}$$

To finish the calculation we pull all the scalars out of the cross porducts,

$$\vec{L} = \left(rm\frac{dr}{dt}\right)(\hat{\mathbf{r}}\times\hat{\mathbf{r}}) + \left(mr^2\frac{d\theta}{dt}\right)(\hat{\mathbf{r}}\times\hat{\theta}), \tag{4.60}$$

and then we note that

$$\begin{aligned} \hat{\mathbf{r}}\times\hat{\mathbf{r}} &= 0, && (4.61) \\ \hat{\mathbf{r}}\times\hat{\theta} &= \hat{\mathbf{z}}. && (4.62) \end{aligned}$$

Thus we find that the angular momentum is given by

$$\vec{L} = \left(mr^2 \frac{d\theta}{dt} \right) \hat{\mathbf{z}}. \tag{4.63}$$

Comparing Eq. (4.56) with Eq. (4.63), we see that

$$\frac{dA}{dt} = \frac{1}{2m} (\vec{L} \cdot \hat{\mathbf{z}}), \tag{4.64}$$

so that conservation of angular momentum ($\vec{L}$ = constant) implies that dA/dt is a constant—the equal area law.

To go further in deriving Kepler's laws we need to know about the actual forces between the sun and the planets. You probably know that one of Newton's great triumphs was to realize that if gravity obeys the "inverse square law," then the rate at which the moon is falling toward the earth as it orbits is consistent with the rate at which objects we can hold in our hands fall toward the ground. In modern language we say that the potential energy for two masses M and m separated by a distance r is given by

$$V(r) = -\frac{GMm}{r}, \tag{4.65}$$

where G is (appropriately enough) known as Newton's constant. We are interested in the case where m is the mass of a planet and M is the mass of the sun. We choose a coordinate system in which the sun is fixed at the origin.

To understand what happens it is useful to write down the total energy of the system. We have the potential energy explicitly, so we need the kinetic energy. We know that the velocity has two components, one in the radial direction and one in the angular direction,

$$\frac{d\vec{r}}{dt} = \frac{dr}{dt} \hat{\mathbf{r}} + r \frac{d\theta}{dt} \hat{\theta}, \tag{4.66}$$

so that

$$\frac{1}{2} m v^2 \equiv \frac{1}{2} m \left| \frac{d\vec{r}}{dt} \right|^2 = \frac{1}{2} m \left[\left(\frac{dr}{dt} \right)^2 + \left(r \frac{d\theta}{dt} \right)^2 \right]. \tag{4.67}$$

So the total energy of the system, kinetic plus potential, is given by

$$E = \frac{1}{2} m \left[\left(\frac{dr}{dt} \right)^2 + \left(r \frac{d\theta}{dt} \right)^2 \right] - \frac{GMm}{r}. \tag{4.68}$$

But we know that angular momentum is conserved, so we can say something about the term that has $d\theta/dt$ in it:

$$\begin{aligned} L_z &= mr^2\frac{d\theta}{dt} && (4.69)\\ \frac{d\theta}{dt} &= \frac{L_z}{mr^2}. && (4.70) \end{aligned}$$

Substituting into our expression for the total energy this becomes

$$\begin{aligned} E &= \frac{1}{2}m\left[\left(\frac{dr}{dt}\right)^2 + \left(r\frac{L_z}{mr^2}\right)^2\right] - \frac{GMm}{r} && (4.71)\\ &= \frac{1}{2}m\left(\frac{dr}{dt}\right)^2 + \frac{L_z^2}{2mr^2} - \frac{GMm}{r} && (4.72)\\ &= \frac{1}{2}m\left(\frac{dr}{dt}\right)^2 + V_{\text{eff}}(r), && (4.73) \end{aligned}$$

where in the last step we have introduced an "effective potential"

$$V_{\text{eff}}(r) = \frac{L_z^2}{2mr^2} - \frac{GMm}{r}. \qquad (4.74)$$

Notice that by doing this our expression for the total energy comes to look like the energy for motion in *one* dimension (r), with a potential energy that has one part from gravity and one part from the indirect effect of the angular momentum.

Notice that the contribution from angular momentum is positive, and varies as $\sim 1/r^2$. This means that the corresponding force $F = -\partial V/\partial r \sim 1/r$ is positive—it pushes outward along the radius. This force is what we experience when we sit in a car going around a curve: the "centrifugal" force. Imagine that we tie a weight on the end of a string and swing it in a circle over our heads. The string will stay taught, and this must be because there is a force pulling outward; again this is the centrifugal force, and is generated by this special term in the effective potential. Notice that we have eliminated any mention of the angle θ, and in the process have changed the potential energy for motion along the radial direction r. This is a much more general idea.

We often eliminate coordinates in the hope of simplifying things, and try to take account of their effects through an effective potential for the coordinates that we do keep in our description. This is very important in big molecules, for example, where we don't want to keep track of every atom but hope that we can just think about a few things such as the distance

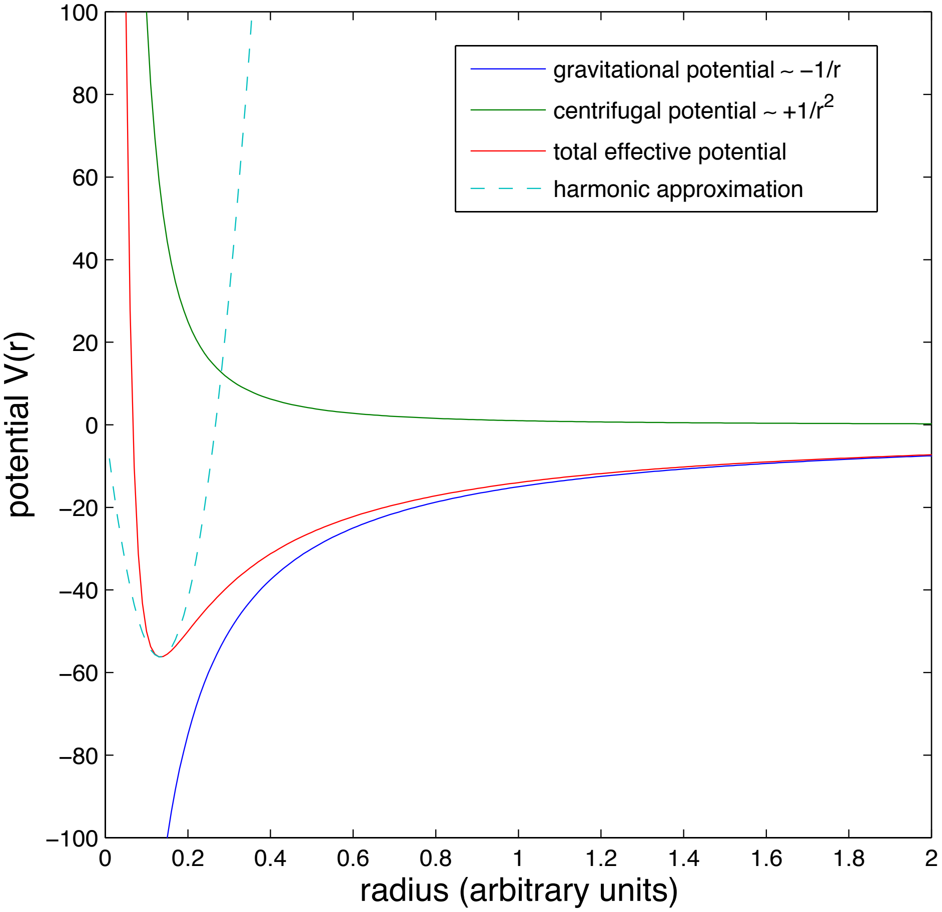


Figure 4.1: Effective potential energy for planetary motion, from Eq (4.74).

between key residues or the angle between two big "arms" of the molecule. It's not at all obvious that this should work, even as an approximation, although in the present case it's actually exact.

Recall that the total energy is the sum of kinetic and potential, and this total is conserved or constant over time. There is a minimum effective potential energy for radial motion, as can be seen in Fig 4.1, If the total energy is equal to this minimum, then there can be no kinetic energy associated with the coordinate r, hence $dr/dt = 0$. Thus for minimum energy orbits, the radius is constant—the planet moves in a circular orbit.

If we look at orbits that have energies just a bit larger than the minimum, we can approximate $V_{\text{eff}}(r)$ as being like a harmonic oscillator. Then the radius should oscillate in time, but time is being marked by going around the orbit, so really the radius will be a sine or cosine function of the angle, and this is the description of an ellipse if it is not too eccentric. In fact if you work harder you can show that the orbits are exactly ellipses for any value of the energy up to some maximum. This is another of Kepler's laws. Once you have the ellipse you can relate its size (the analog of radius for a circle) to the period of the orbit, and this is the last of Kepler's laws.

Notice that if the energy is positive then it is possible for the planet to escape toward $r \to \infty$ at finite velocity, and then the orbit is not bound. But if the total energy is negative, there is no escape, and the radius r moves between two limiting values, namely the points where the total energy intersects the effective potential. We really should say more about all this, but it is treated in many standard texts. [But should add something about rotation curves and dark matter in galaxies!]

4.4 Biological counterpoint

[This section remains to be written. Current students should check on `blackboard` to see if some more informal notes are posted.]