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QUANTUM MECHANIC'S MANUAL

PHYS441, Winter 2020

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Contents

Chapter 1

Introduction

1.1 The Book Notes

Our imagination is stretched to the utmost, not, as in fiction, to imagine things which are not really there, but just to comprehend things which **are** *there.* R.P.Feynman

The point is no longer that quantum mechanics is an extraordinarily (and, for Einstein, unacceptably) peculiar theory, but that the world is an extraordinarily peculiar place. N.D.Mermin

Quantum Mechanics is one of the most amazing accomplishments of the human spirit. It describes **reality**, most of which we never see or sense in any direct way, and it shows how the **illusion** of our everyday life comes about as the 'classical limit'. We really do not have any right to assume that we should be able to calculate as much as we do, so it is a miracle (a loose quote from Einstein: the most incomprehensible thing about Nature is that it *appears* comprehensible).
Note well that I use the words 'describe' and 'calculate'; how much we really *understand'* is a completely different question. We will address this aspect of quantum physics as much as is possible at this stage, but the fact is that you will have to learn a great deal before much speculation on quantum philosophy becomes useful. Some people rejoice in new and strange notions, others get discouraged. If you will find yourself in the latter category, keep in mind that it is worth it: among the countless thousands of experiments on atomic, molecular, condensed matter, nuclear and particle physics (and of course much of chemistry, even astrophysics) there is not a single piece of experimental data in existence which would contradict Quantum Mechanics.

If everything goes well, this Manual – enhanced by your personal notes from lectures and study – should become a comprehensive text for this course, as well as your aide-memoire. It reflects my ideas about the order of presentation and level of rigour that should be applied at this time. Some topics are mentioned with only a few comments and/or with a summary of key concepts. On the other hand, selected subjects are treated in detail (still, in a non-verbose way). As a rule, it should be possible for you to fill in all the missing steps (and, in general, you will find it very useful to do that !). Used properly, in combination with the Peleg book, should be an efficient way for each of you to become a Certified Quantum Mechanic :-)

Any comments on the Manual (or on anything else) will be much appreciated.

1.2 Instructors

Lecture Instructor: Vladi Chaloupka, Professor of Physics, PAB room B143, vladi@uw.edu, office hours Mon&Wed 6:00-6:45 PM and after class

Teaching Assistant: Tyler Blanton, Physics graduate stdent/PHD candidate, PAB room B143, blanton1@uw.edu, office hours Mon&Wed 6:00-7:0 PM and by appointment

1.3 (Text)books

1) "Quantum Mechanics" by Yoav Peleg, Reuven Pnini and Elyahu Zaarur 2nd edition (joined by Hecht as a co-author, strangely writing the new prefacthe theory (that's why you have to come to class) but very rich in solved examples. It is, by far, the best value for your money (about $15 at Amazon and elsewhere) and it contains an abundance of problems solved in complete detail.

2) These Lecture Notes, annotated by you at the lecture and when studying later. Those of you who find the Lecture Notes too compact are encouraged to browse the bibliography below, and select a text that you like – much is also available on the web. I used the first three books listed (Griffiths, Bransden/Joachain and Gasiorowicz) in this course in the past, so they are recommended. In general, I follow somewhat different sequence from most textbooks – for good reasons, I think. The ability to find a detailed explanation in a book or online when you need it is one of the skills you will need in your studies, as well as in your subsequent career.

Optional texts:
Griffiths: Introduction to Quantum Mechanics, 2nd edition. Very popular text, written almost as a transcript of actual lectures. (example: *"..... Physically realizable states correspond to the 'square-integrable' solution to Schroedinger equation. But wait a minute! Suppose I have normalized the wave function ...."*) If you like to be talked to, then this is a book for you. Myself, I cringe at times ....

Bransden/Joachain: Quantum mechanics (2nd ed.) I used this text previously, and covered Chapters 1-6, with some omissions and some additions. Chapter 1 is a very useful recap of Modern Physics missing from the other two books. Very good chapters on various applications of Quantum Physics (this might be useful for PHYS 541).

Gasiorowicz: Quantum Physics (3rd ed. Wiley 2003). Used in the past. Now includes many online appendices, but I liked the 1st edition better ...

and of course, there is always the (almost) timeless and (almost) perfect classic: Feynman Lectures on Physics!!!

Super-optional readings: Koestler's *Sleepwalkers* is the most fascinating book on Science I ever read. The concepts of a scientist as a sleepwalker has been taken over by John Bell of the Bell Inequality fame, and is described beautifully in his "Speakable and Unspeakable in Quantum Mechanics."

Hofstadter's *Godel Escher Bach* is, still, the best account of the deep connections between Sciences (including mathematics) and Art. It does not require any prerequisites, but some pages may take you half an hour or more ... At the end, you will be a better (at least a better-educated) person.

And last (and least): a "From Bach to Einstein and Beyond" - a Big Book in progress by yours truly. Any comments will be most welcome – this is what I am really concerned about these days ... And to get to know your Instructor up close and personal, you may want to have a look at the first chapter – see two attachments to my email.

1.4 General notes

This course is a core (required) course for participants in the "MS in Applied Physics" program. Some resulting features of the course may be attractive to a wider audience, including students from outside the Physics Department. Since many of our evening students have been out of school for several years, both this course and the EM course (PHYS543) are designed to help re-fresh some possibly forgotten math and physics skills. This means that the subject matter is covered "from scratch", and extensive help is available to students who might need it. At the same time, since the audience is more mature and better motivated than typical Junior class, the tempo is brisk, and the level is quite rigorous. In short, you can expect to learn a lot (if you are willing to work on it.)

Approach to Math: It has been said:

A proof convinces a reasonable man.
A rigorous proof convinces an unreasonable man.

This course will be "rigorous" in a different way. The proofs which will be given, rather than skipped, will be given not to convince you, but because they are illuminating and/or useful on their own. It will be "rigorous" not in the sense of splitting hair and enumerating all possible pathological cases when a theorem does not apply (most pathological cases don't really occur in Nature / Physics), but in the sense that we will try to really understand everything, or clearly recognize what it is that we don't understand.

1.5 Homework, Exams and Grading

There will be some problems assigned/suggested in this Manual as well as during lectures, but each student should self-assign additional problems from Peleg book. It is VERY IMPORTANT to attempt each and every problem BEFORE looking at the solutions (I recommend

covering each solution with a sheet of paper to start with, and then use the “strip technique” as explained at lecture ...).
It is of utmost importance not to get behind.

The philosophy of this course is

1) ”you will get out ot it what you put in”

2) To provide enough challenge to satisfy everyone, here will be more material presented than can be expected even from a bright and determined student.

3) To serve students with perhaps insufficient preparation, all important topics will be covered from scratch.

I will determine your course grade after I examine

1) 40 % of your final grade. Your Quantum Diary covering all work you did for the course (PLEASE TYPE (preferred) or WRITE LEGIBLY – I cannot grade what I cannot read)

Typical entry might be:

date, number of hours spent, on what: studied Manual Chapter/section and found .., studied Peleg text section(s) XXX, Peleg problem(s) YYY; visited office hours and understood ZZZ, ...

2) 40 % of your final grade. Your copy of the PDF of this Manual personalized/annotated by your conclusions, comments, ideas, questions ... Use mainly brief sticky notes, and corresponding highlighted text. Put the more verbose into your Quantum Diary. Typical sticky note might be: ”Where did this came from?” (and if you asked me or the TA, add second sticky Note like ”TA/Vladi/friend explained). Also: ”Needs more explanation”, ”Typo” for a typo etc. Also feel free to say this of that was interesting, or just an exclamation point etc.

For your annotations please use the Adobe Reader DC or equivalent (enabling text highlighting/underlining, sticky notes, and the identification of the writer (i.e. you).

3) There will be a Final Exam on the Things to Take Away from the course; it will count for 20 % of your final grade. The ”Things” you need to understand and may be asked to explain and discuss will be emphasized in Lectures.

The grading will be pretty loose, reflecting the course philosophy. In case of any doubt about acceptability of your work please do not hesitate to show me what you are doing as we go along.

NOTE: I will make an effort to lecture from our classroom at the UW as often as possible. However, there will be times where I will have to lecture from home and broadcast the lecture using the ZOOM system. I will send an EMAIL out as soon as I learn this will happen. And in fact, ALL lectures will be available on ZOOM in real time as well as recorded for later viewing. Some students might find it useful to come to the UW for every lecture, to benefit with the interaction with their peers.

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     PHYS441     Tentative Schedule      Winter2020

Jan    6         Ch. 1,2 Introduction to course and to Quantum Physics
       8
-------------------------------------------------------------------------------
      13         Ch. 10 delta function, Fourier, complex, vectors/matrices
      15         Ch. 3  Quantum Wave Mechanics
-------------------------------------------------------------------------------
      20  MLK Day
      22
-------------------------------------------------------------------------------
      27         Ch. 4  Quantum Mechanics I
      28
-------------------------------------------------------------------------------
Feb    3
       5          Ch.5  Quantum Mechanics II: Hilbert space
-------------------------------------------------------------------------------
      10
      12
-------------------------------------------------------------------------------
      17     Presidents Day
      19
-------------------------------------------------------------------------------
      24          Ch. 6  Angular Momentum
      26
-------------------------------------------------------------------------------
Mar    2          Ch. 7  Atoms
       4     reserve
-------------------------------------------------------------------------------
       9          Ch. 8  Bell Inequality, Quantum Computing,
      11     Grand Finale
-------------------------------------------------------------------------------
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Course website: http://faculty.washington.edu/vladi/PHYS441

Chapter 2

Introduction to Quantum Physics

2.1 Experimental evidence for Quantum Physics

The amount of experimental evidence for quantum physics is overwhelming. As noted above, *all* available data agrees with quantum mechanics, and much of our civilization is actually based on it. In general, I am not a great advocate of a historical approach to science, but there are some foundational experiments of extreme significance and great beauty:

By the end of the 19th century physics has achieved amazing successes:

– Newton, building on contributions of Kepler and Galileo, provided the foundations. unifying everyday mechanics with the celestial motion.

– Maxwell, in a spectacular accomplishment, unified electricity, magnetism and optics. He predicted that a disturbance of the electromagnetic field should travel at a speed of $1/\sqrt{\epsilon_0\mu_0} \sim 3 \times 10^8 m/s$. In a truly historic moment, he learned, upon returning from his country house, that astronomers just measured speed of light to be $\sim 3 \times 10^8 m/s$.

However, some even more dramatic and far-reaching developments were awaiting around the corner of the 20th century.

2.1.1 The humble black body.

A black body is an object that does not reflect any light illuminating it – it absorbs everything. But by absorbing the EM energy it gains it and therefore it emits EM energy back, in general with a different spectrum. The classical realization has been a cavity with its inner walls maintained at a constant temperature T. After some time an equilibrium is established, where the energy received each second is equal to the energy radiated. The radiation in the cavity can studied by analyzing the radiation coming from a small hole (see Figure 2.1)

It was soon recognized that the equilibrium is characterized by the temperature T the body achieves, and – what is more interesting – the spectrum of that radiation depends only on

T and on the frequency f[1] (or equivalentlyλ[2] on the wavelength

$$u(f,T) = \frac{c}{f^2} u(\lambda, T)$$

The independence of the energy spectrum on the blackbody details shows that this is an important, universal aspect of the thermodynamics, and therefore a significant effort centered on find the expression for the energy density $u(f,T)$

Using very solid classical physics arguments, Rayleigh derived the expression

$$u(f,T) = \frac{8\pi f^2}{c^3} kT \tag{2.1}$$

and it was a disaster – see Figure 2.2. It agreed with the experimental data for low frequencies, but it literally exploded, unphysically, at high f. Because no one was able to find fault with Rayleigh reasoning, it became "the ultraviolet catastrophe".

On the other hand, Wien proposed an expression he found (based on a model that is no longer of interest)

$$u(f,T) = a f^3 e^{-bf/T} \tag{2.2}$$

and this, with the right choice of the adjustable parameters a and b worked quite well (see Figure 2.2). The agreement at high frequency was now perfect (no UV catastrophe!) but now the low frequencies were showing a small but definite and unacceptable discrepancy.

So at the very beginning of the twentieth century there were two formulas; one OK at high frequencies, the other one at low f. And in the year 1900, in a singular development in physics, Max Planck discovered the correct formula by purely mathematical trial and error:

$$u(f,T) = \frac{8\pi h}{c^3} \frac{f^3}{e^{hf/kT} - 1} \tag{2.3}$$

He *knew* it was correct because it agreed with the experimental data so excellently and over the full range of the variables. In addition, it beautifully made the transition between the Rayleigh and the Wien formulas (see Figure 2.2). So now Planck set out to find out what physics assumptions would yield his result.

After two months of work, he found and – as he was an old-school, careful and conservative[3] physicist – reluctantly accepted the result: it appeared that the cavity walls emit EM radiation in "quanta" of energy hf, 2hf, 3hf, ...nhf - and nothing in between. As a consequence, the Boltzman classical average of energy

$$< E >= \int E.Prob(E) dE = \int E \frac{e^{-E/kT}}{\int e^{-E/kT} dE} dE \tag{2.4}$$

[1]NOTE: I refuse the Greek ν for frequency: just think of the equation $\nu = v/\lambda$ (especially when handwritten ...)

[2]Plotting the dependence on the wavelength seems more familiar; the dependence of frequency makes clear the physics contents of the final Planck solution (see below).

[3]I say "conservative" in the best sense of the word; more about this in chapter XXX

becomes (with $x = hf/kT$ where h is the Planck constant and k is the Boltzman constant)

$$< E >= \frac{\sum_{n=0}^{\infty} nxe^{-nx}}{\sum_{n=0}^{\infty} e^{-nx}} = \frac{-x\frac{d}{dx}\sum_{n=0}^{\infty} e^{-nx}}{\sum_{n=0}^{\infty} e^{-nx}} = x\frac{e^{-x}}{1-e^{-x}} = \frac{x}{e^{x}-1} \tag{2.5}$$

which, when multiplied by the classical density of states $\frac{8\pi f^2}{c^3}$, becomes the Planck formula. And it is a nice exercise to show it is indeed a smooth transition between Rayleigh and Wien:

$$\lim_{x->0} eq.2.3 = eq.2.1$$

$$\lim_{x->\infty} eq.2.3 = eq.2.2$$

It also is a simple and very nice exercise on integral calculus. Normally, the definite integral is defined as the surface beneath the curve $y(x)$ calculated as a limit of a sum, i.e. the sum is an approximation. But sometimes Nature insists on using the sum, and it is the integral that is an approximation. Equations 2.4 and 2.5, illustrated on Figure 2.4, show how this comes about.

And finally, and remarkably, the Planck formula does not have any free parameter – not even for overall normalization (just two universal constants: the Planck constant h and the Boltzmann constant k). Both dependencies are quite dramatic (for the h on frequency, for the k on temperature, so Planck was able to determine both values with remarkable accuracy).

Note: physicists often use the value of the "hbar" defined as

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

Summary

This was the first crack in the safe where Nature kept the quantum from us, and Max Planck is immortal for making the breakthrough.

2.1.2 From Black Body to Blackbody to the Big Bang

As fundamental as the blackbody was for the origin of Quantum Physics, there is more – much more.

- Relic from the Big Bang.

  As early as 1948, based on not much more than the data on present-day abundances of the light elements (H, D, ...) George Gamow and collaborators predicted that a Big Bang should have left behind a relic of very low temperature radiation. In 1955, in an experiment aimed at reducing the noise interfering with the signals from the first active communication satellites, Penzias and Wilson observed a persistent excess of radiation around the temperature of about 3 K. Fortunately, they knew that Jim Peebles and collaborators were looking for the Big Bang relics in that temperature range. So they persisted, and published their results; Peebles and Co. published the interpretation in the same issue of the journal, and the age of experimental cosmology was born. Penzias and Wilson received a Nobel Prize in 1978; Jim Peebles continued a remarkable involvement in cosmology and received an overdue, much deserved Nobel Prize in 2019.

- The COBE spacecraft experiment

  Experimental cosmology continued mostly with high altitude balloons, and came of age with the launch of the COBE satellite in 1989. The first great result was obtained very soon: their measurement on the spectrum of the "relic" - now officially called the Cosmic Microwave Background Radiation (CMBR) produced a fantastic agreement with the Planck formula – see Figure 2.5. By now it was very difficult to think of any other origin of the CMBR than a hot Big Bang. Therefore, this is a good time for a brief overview.

  Figure 2.7 shows the (by now) standard chronology of the Big Bang showing how the part of the Universe currently observable by us started extremely small and extremely hot, and in some 13 billions years gradually cooled down to the present temperature of 3K and expanded to the present radius of some 42 light years (this is more than 13 billion due to the Universe expansion). It is a very busy diagram, and one can (and should) spend a lot of time inspecting and reflecting its many features. It is mind boggling that we can interpolate our knowledge over so many orders of magnitude, and it us only natural that one′s degree of confidence decreases as we go closer and closer to the Big Bang itself. Here, we start very conservatively at the end of the period of nucleosynthesis that lasted from about 10^{-10} to 10^{-9} seconds (it sounds really weird to use the word "lasted" in that sentence ...). The Universe was about one second old and "only" 13 million[sic] light years across and contained a mix of protons, neutrons, electrons, neutrinos and photons violently agitated at temperature of 10 billion K. And then light nuclei were produced, and nothing much happened for about 350 000 years – Universe was gradually expanding and cooling down. And then, quite suddenly, something dramatic happened. As the temperature decreased to about 3,000 K, electrons became for the first time able to combine with the nuclei to produce neutral atoms, and the Universe became transparent. For some obscure reason, this is called "recombination" but those electron and nuclei were never combined previously ... Figures 2.11 and 2.8 illustrate the process.

  The 3,000 K photons then traveled unimpeded and kept cooling by the continuing expansion until they reached their todays's temperature T=2.7 K. This is the Cosmic Microwave Background Radiation that Gamow (and others) predicted, Penzias and Wislon (and others) observed, and the COBE experiment could begin to investigate in detail. We already mentioned that their very first result (said to have been achieved in the first nine minutes!) was finding a spectacular agreement of the spectrum with the Planck black body formula. The whole Universe was a black body when CMBR was emitted because it originated in the whole Universe that is an isolated system by definition, and all its constituents were in thermal equilibrium because the expansion rate was much slower than the rate of the thermal motion. In fact, the CMBR is the best black body found in the Universe.

- The absolute speed of Earth. By 1992 COBE accumulated enough data for a detailed investigation of the CMBR, Figure 2.6 show that the results were almost too good to be true:

  a) the temperature was uniformly 2.7 K in all directions. This was great news for the theory: "we" were originally "in the middle" of everything (because everything was in the middle of everything). Now we are at the center of a "Hubbel bubble" of the radius of the observable Universe, and CMBR comes uniformly in as it has been emitted from the inner surface of a sphere called the surface of last scattering (see Figure 2.9).

  b) when restricting the data a narrow temperature range of $\pm 3.5 mK$ a dipole signal appeared, consistent with the Earth moving through the CMBR background with a speed about 600 km/s. Special relativity is still valid, but clearly there is one reference frame that is more equal than the others[4]:-)

  c) And finally, the great prize: when removing the dipole signal and restricting the data to $\pm 20 \mu K$ [sic !!!] there appeared a signal from the radiation of our own galaxy – which is not much more than a nuissance. But the data out of the galactic plane show a clear variation of randomly looking cold and hot spots. This was the Holy Grail, the hope of cosmologists which came to be fulfilled. Of course, the Nobel Prizes did not fail to come (to Mather and Smoot, the COBE leaders, in 2006).

- The (rare) definitive experiment.

  The COBE experiment was followed up – with significantly more detailed results – by the WMAP project, and then by a definitive experiment called – appropriately – Planck. The cumulative progress can be seen on Figure 2.10. The pattern of cold and hot spots turned out to be anything but random. In the manner of decomposing a sound signal into contributions of various harmonics, one can similarly express the two-dimensional pattern into different "spherical harmonics" that are called "multipoles". Naturally, the subsequent experiments show more and more details, so we show on Figure 2.12 the results from the Planck experiment. And this is the real Holy Grail. Nature has been kind to us: the peaks of the distribution contain priceless information on various cosmological models and their parameters.

  The peaks seen on the Figure are called "acoustic peaks". It may sound strange that we speak of acoustics in the emptiness of space. But the space was not empty when CMBR was emitted – as you can see from Figure 2.7 the density was considerable, and it was sufficient to enable mechanical waves fully analogous to sound waves in air. But what is important is the amount of information that is provided by the exact locations

[4]Expanding on this and previous paragraph: the emission of CMBR happened everywhere at the same time, and it was a very brief (relarively speaking :-) flash emitted at about (13,000,000,000 + 300) years after the Big Bang. We keep seeing it as if it kept happening, but this is an illusion due to the CMBR photons coming at us from larger and larger distances.

and heights of the peaks. As a dramatic example, it was possible to determine from the spectrum that the metric of the observable Universe is not curved but compatible with flat. This means that the whole Universe is very much larger than our observable Universe, maybe infinite. It is awe inspiring that we can meaningfully discuss the whole Universe that we have never seen and will never see ...

I called the experiment definitive because its determination of the acoustic peaks cannot be improved. The resolution of the peaks is limited by the physical effects along the path of the CMBR photons from the surface of last scattering to us. When the resolution of the measurements exceeds this limit, any additional measurement will not change the results (unless, of course, the Planck team committed some grave errors, which is very unlikely). So the experiments is definitive and this is rare (and very valuable).

And finally: I find it remarkable to what degree the theory and the experiment co-operated in achieving the truly breathtaking results that we have discussed. Often it happens that the theory follows the experiment, and the work of the theorists may then have the nature of an after-the-fact postdiction. This significantly reduces the power of any claim that the successful experiments "confirmed" the theory. A dramatic example of the impressive lead of the theory in cosmology can be seen on Figure 2.13.

In fact, an even much more dramatic example concerns the cosmic inflation. So far we refrained from discussing it because limiting ourselves to the more reliable concepts seemed are-inspiring enough. Inflation refers to the possibility that the Universe went from initial size of e.g. 10^{-10} to a size of e.g. 10^{+15} meters, within the time of e.g. 10^{-28} seconds; then the "regular" Big Bang followed (well, this would make the Big Bang look not so spectacular, after all -:) This has been motivated by the hope that it would remove some of the remaining difficulties with the theory. It so happens that some (many?) cosmologists now claim that the data from the Black Body research provide (or will provide, when polarization measurements improve) experimental evidence that inflation has in fact happened. As I remarked when discussing the metric of the "whole Universe": the mere fact that we can meaningfully discuss the cosmic inflation is mind boggling.

2.1.3 Max Planck Conclusions, in his own words

Near the end of the Prelude I noted the hope in an eventual recovery of my youthful optimism in our young people, children and grandchildren. Stories like the one I told you in this chapter reinforce that hope. I will close with the words of the Great Man himself:

"Science enhances the moral value of life, because it furthers a love of truth and reverence; love of truth displaying itself in the constant endeavor to arrive at a more exact knowledge of the world of mind and matter around us, and reverence, because every advance in knowledge brings us face to face with the mystery of our own being.

2.1.4 blackbody spectrum summarized

The dependence of the "blackbody spectrum" on wavelength requires quantization of energy levels of electromagnetic radiation inside the black body cavity, with

$$E \;=\; hf \qquad h \;=\; 6.6\; 10^{-34}\; J.s$$

The "Planck constant" is a fundamental property of Nature, and honors the scientist who discovered it (in addition to the Nobel prize he received).

Note the time sequence of Planck's discovery (correct formula first, its derivation two months later), and do not miss a useful lesson on integration and averaging.

A fascinating example of black-body radiation is the "cosmic background" of radiation emitted when, after the Big Bang, radiation "decoupled" from matter. This happened when Universe was about 400,000 years old, and the temperature was 3000 K. Since then, the expansion of the Universe by a factor of about 1,000 has cooled down the radiation by the same factor to about 3 K today. The precise measurements of the "ripples" in the cosmic background are starting to provide some incredibly detailed evidence on the early Universe (as well as information on our *"absolute"* speed).

2.1.5 photoelectric effect

The second foundational quantum effect was discovered by Hertz in 1887, studied by Lenard[5] and interpreted by Einstein in 2005.

Electrons are ejected from an anode by a stream of photons, and collected by a cathode (see Figure 2.14). The main results are

1) The collected current depends on the light intensity, but the "stopping potential" (necessary to prevent any electrons from reaching the cathode) does not

2) On the other hand, the stopping potential does depend on the frequency of the light used.

$$eV \;+ W = \; hf$$

where W is the "work function" of the particular metal the anode is made of – only voltage above this value can accelerate the electrons. And the constant h "happens to be' the same number as the h in a) as well as below. This might remind you of Maxwell's triumph showing that his $1/\sqrt{\epsilon\mu}$ equaled the speed of light as measured directly.

Explanation of the photoeffect is what Einstein received his Nobel Prize for[6]: radiation of frequency f consists of quanta called photons, each of energy hf. You should see, and be able to show to anyone, the extraordinary beauty of the reasoning.

[5]Lenard won the Physics Nobel Prize for his research. This did not prevent him from becoming a fervent Nazi supporter, together with Johannes Stark, another Nobelist.

[6]I believe he should have received at least another Physics Nobel for General Relativity, plus a Peace Nobel Prize ...

2.1.6 Compton effect:

photon-electron elastic scattering, with the "recoil" photon showing lower frequency than the initial photon. This shows that a photon is a "particle" with energy and momentum

$$E = hf \qquad p = E/c$$

Recall the general formula

$$E = \sqrt{m^2c^4 + p^2c^2}$$

with the special cases (HW!) of
a) rest
b) non-relativistic motion (yielding the familiar expression for the kinetic energy)
c) ultra-relativistic case (i.e. EM)

2.1.7 diffraction of electrons

although they are generally considered to be particles, they exhibit diffraction as a wave with the wavelength

$$\lambda = h/p$$

Note the serendipitous role of broken equipment, and also the family symbolism:

J.J.Thomson (Nobel prize 1906 for showing quantum nature of electricity)

G.P.Thomson (Nobel prize 1937 for showing wave nature of electrons)

2.1.8 quantization of physical quantities:

atomic spectra: the spectra of light emitted by excited atoms are quantized as

$$hf_{ab} = E_b - E_a$$

where, as discovered later, E_b and E_a are the energies of the initial and final state (i.e. there was a "quantum jump" from state a to state b). We will be able to calculate that soon enough.

Stern-Gerlach experiment: the deflection of particles going through inhomogeneous magnetic field are quantized as if the had the angular momentum projection quantized as:

$$L_z = mh/2\pi = m\hbar$$

where m is an integer; see Figure 2.15

2.2 The Puzzle Illustrated by the Double Slit Experiment:

(Feynman Vol. III,1.-3.) see our Figure Figure 2.16

To fully appreciate the Puzzle, you should try to 'comprehend' that if you **open** the slit B, electrons will **stop arriving** at point P !

HW: impress your friends with this, the Central Mystery of Quantum Physics, using a modified version of the double-slit experiment using the "Mach-Zehnder" interferometer. This not only illustrates the puzzle directly and quantitatively, but it also serves as an example of the central role that interferometry (looking at a tiny *differences*) plays in modern physics.

2.2.1 The Interferometer

Light impinges on a half-silvered mirror BS (BS is for 'Beam Splitter" !). The rest of the spectrometer consists of two ordinary mirrors M1 and M2, detectors D1, D2 and D1' and a screen, as indicated on Figure 2.21. As discussed in the Figure caption, the beam splitter splits the beam in a very remarkable way.
In addition: When we do something to one path and not to the other one as indicated by "B=?"(the simplest is to introduce a gradual delay along path 1, or magnetic field with which we can gradually change the phase of the beam) the whole spectrum of fringes gradually shifts.

The results show a big puzzle: when only one detector is in place, we observe that each and every particle came through path 1 or path 2. But without the detectors we observe the interference, as if SOMETHING passed through BOTH paths. But what is that "something' ???

We obtain similar results using all particles (photons, neutrons, atoms, even molecules). And note that this is not some weird quantum theory: these experimental facts will have to be explain by the present or ANY future theory (recall the quotes on top of the first page).

Using particles traveling slower than light, we can have fun of thinking about the ontology when we place. The path one detector in the position D_1'. Whenever this detector does not detect the particle when predicted, we know that (and exactly when) will the detector D_2 hit. What is the ontological status of the particles between the non-detection by D1' and detection by D2?

And last but not least: the particles are detected as single impacts, no matter how far from the source, and the interference effects subsist when then flux of particle is so low that they come literally "on by one" (see Figure Figure 2.22).

So what happens?

Some say: well, the two particles 'simply come through both paths at the same time. That seems very difficult. Each copy of c. the particle behaves like the whole particle, with its full energy, momentum etc. And it is easy to extend the setup so that the initial beam is split into many beams, even infinitely many, even uncountably infinitely many.

In an apparent act of desperation, believers in the Many Worlds interpretation double down: with every single quantum decision to be made anywhere, the whole Universe splits into as many Universes as there are the possible options for that quantum event.

We have something real simple, say the proponent of the Transactional Interpretation: any single quantum event simply sends faster-then-light to all possible quantum partners and the deceision is made depending on which transaction prevails ...

With all due respect to my learned colleagues, all these cures seem (much) worse than the disease.

As we shall see, the standard interpretation of our present theory (quantum mechanics) claims that this question is meaningless. The formalism allows us to correctly calculate the probabilities of the outcome of any experiment we can perform, the experiments discussed above are different experiments, and "what really happened" is, at best, a question for philosophers (while the "real physicists" say: "Shut up and calculate" :-).

On the other hand, some of us say: just wait a minute (or a century or two...)! More on this in Lectures ...

2.3 Fundamentals of Quantum Physics

Summary of experiments

1) wave-particle duality

	bullets	water waves	electrons	EM waves
lumps(quanta) ?	yes	no	yes	YES
interference ?	no	yes	YES	yes

(the answers in upper case are the essence of the quantum-mechanical particle-wave duality)

2) Many physical quantities are "quantized".

2.3.1 The Quantum Mechanical Solution of the Puzzle:

Planck (1901) : $E = hf$ to explain blackbody spectrum

Einstein (1905) : $p = E/c = hf/c = h/\lambda$ to explain photoelectric effect

deBroglie (1925) : a (complex) wave with $\lambda = h/p$ also for electrons etc.

(all of the above with the same value of the Planck constant $h =$)

Born (1927) : probabilistic interpretation of ψ

momentum p**, energy** E $\Longleftrightarrow$ **complex** $\psi(x,t)$ **with wavelength** $\lambda = h/p$ **and period** $T = h/E$

We shall see how boundary conditions impose quantization. A bit later, we shall see how all this is embedded in the abstract, elegant theory of Quantum Physics in Hilbert Space.

2.3.2 Particle in a potential "box"

Already at this stage we can do some quite fundamental physics. Consider a very simple but very useful "playground" of Quantum Mechanics (see Figure 4.2). Particle of mass m is confined in a potential $V(x) = 0$ for $0 < x < a$ and $V(x) = \infty$ outside.
Standing waves with

$$L = n\lambda_n/2$$

immediately yield quantization of energy

$$E_n = n^2 E_1$$

where $E_1 = h^2/8mL^2 \neq 0$

This is our first encounter with quantization as consequence of the boundary conditions. The hydrogen atom will turn out to be just like this (only a little more complicated mathematically). The remarkable, highly non-classical result that the ground energy is not zero will turn out to be required by the Uncertainty Principle.

2.3.3 Development of quantum physics continued

Born rule elaborated

It would be hard to overestimate the importance of the Born rule giving the correct interpretation of the wave function. It is interesting to note that Born, in his Nobel lecture, gave credit to Albert Einstein (so much for "Einstein was wrong" etc ...).

$\mid \psi(x) \mid^2 dx \;\equiv$ probability of finding the particle in $(x, x + dx)$

$\int_a^b \mid \psi(x) \mid^2 dx \;\equiv$ probability of finding the particle in (a, b)

$\mid \psi(x) \mid^2 \equiv$ probability **density**

$\psi(x) \;\equiv$ probability **amplitude** or the "**possibility** wave"

for a discrete case, $|\psi_i|^2$ is the probability of the i-th outcome

several **distinguishable** alternatives: add **probabilities**

for several **indistinguishable** alternatives: add **probability amplitudes** or **possibilities** or **wave functions**

NOTE: When you think about it, the alternatives to get a given (i.e. fully specified) quantum state from a given (fully specified) initial state are ALWAYS indistinguishable. Failure to appreciate this is at the origin of many published papers.

2.4 Figures

Figure 2.1: Commercially available blackbody. With a heater (or cooler) and temperature lock.

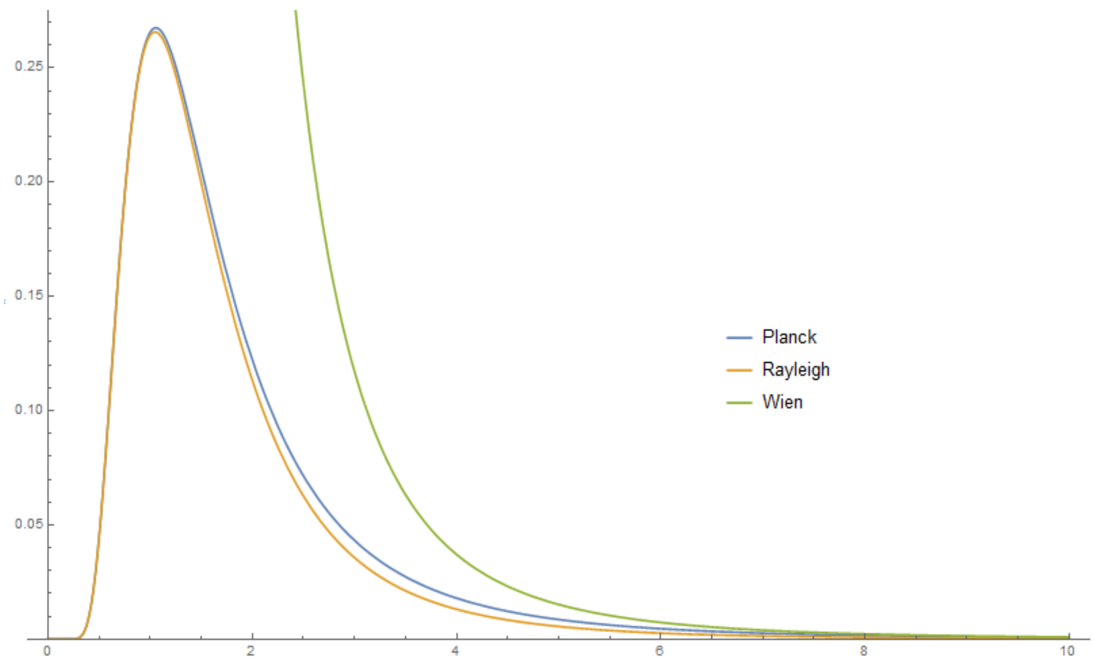

Figure 2.2: Horizontal is the wavelength in mm. The UV catastrophe is obvious. To appreciate the low frequency behavior see the LogLog plot next.

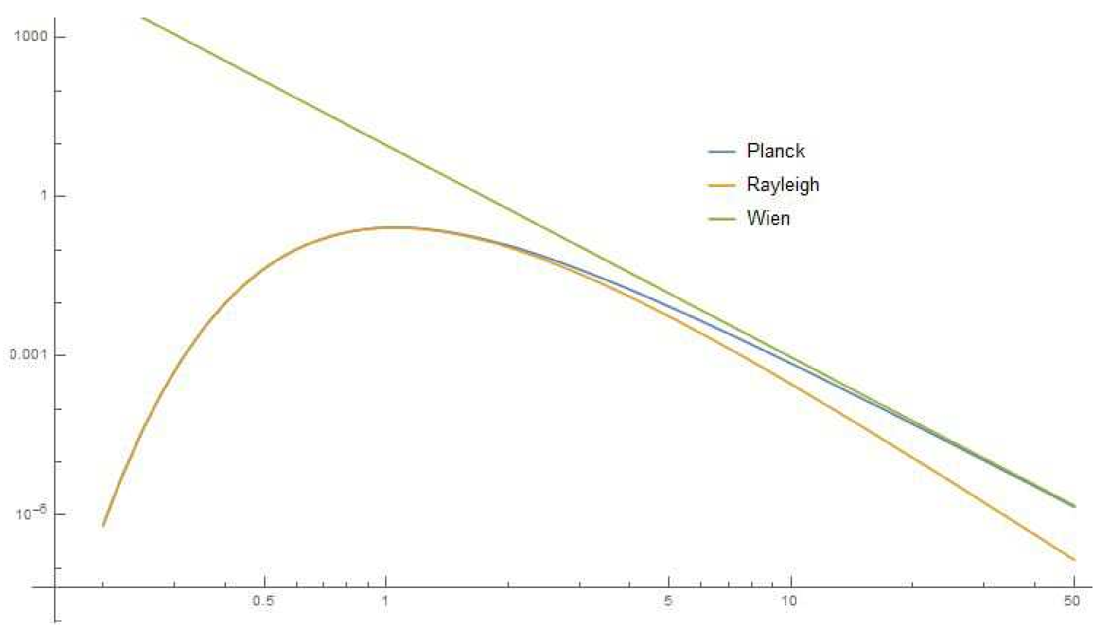

Figure 2.3: LogLog of previous plot. I am mesmerized by this graph :-)

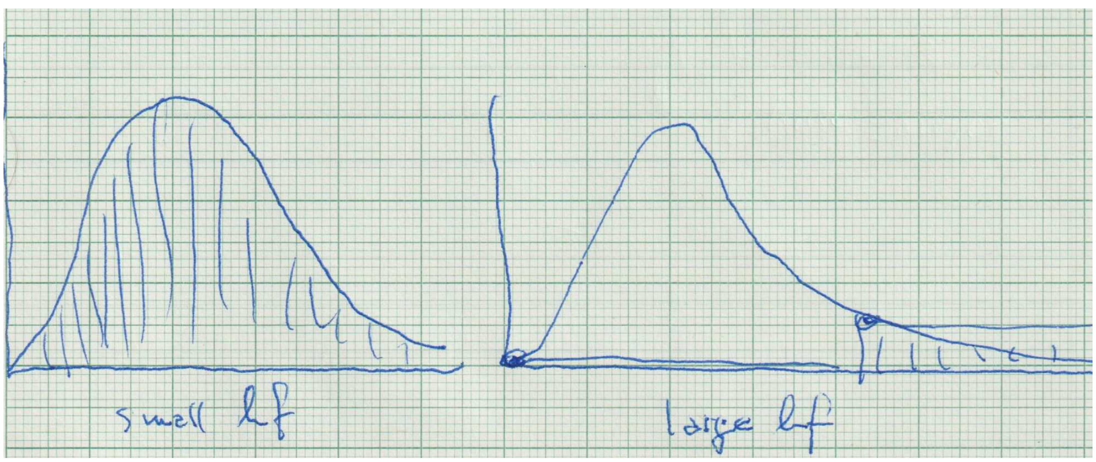

Figure 2.4: An elementary integral/sum lesson.

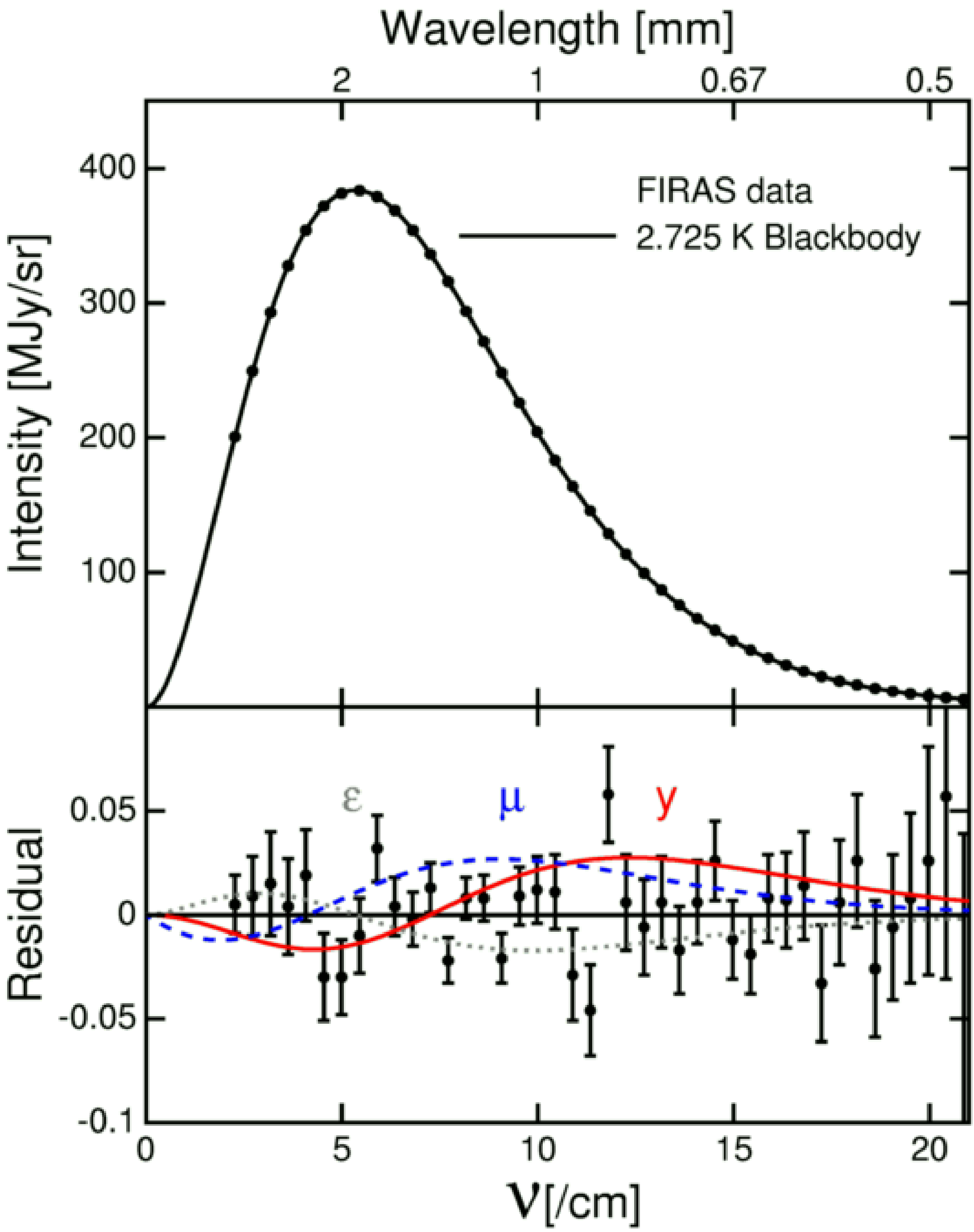

Figure 2.5: The error bars are smaller than the thickness of the line. Magnified at the bottom; the curves are no longer relevant.

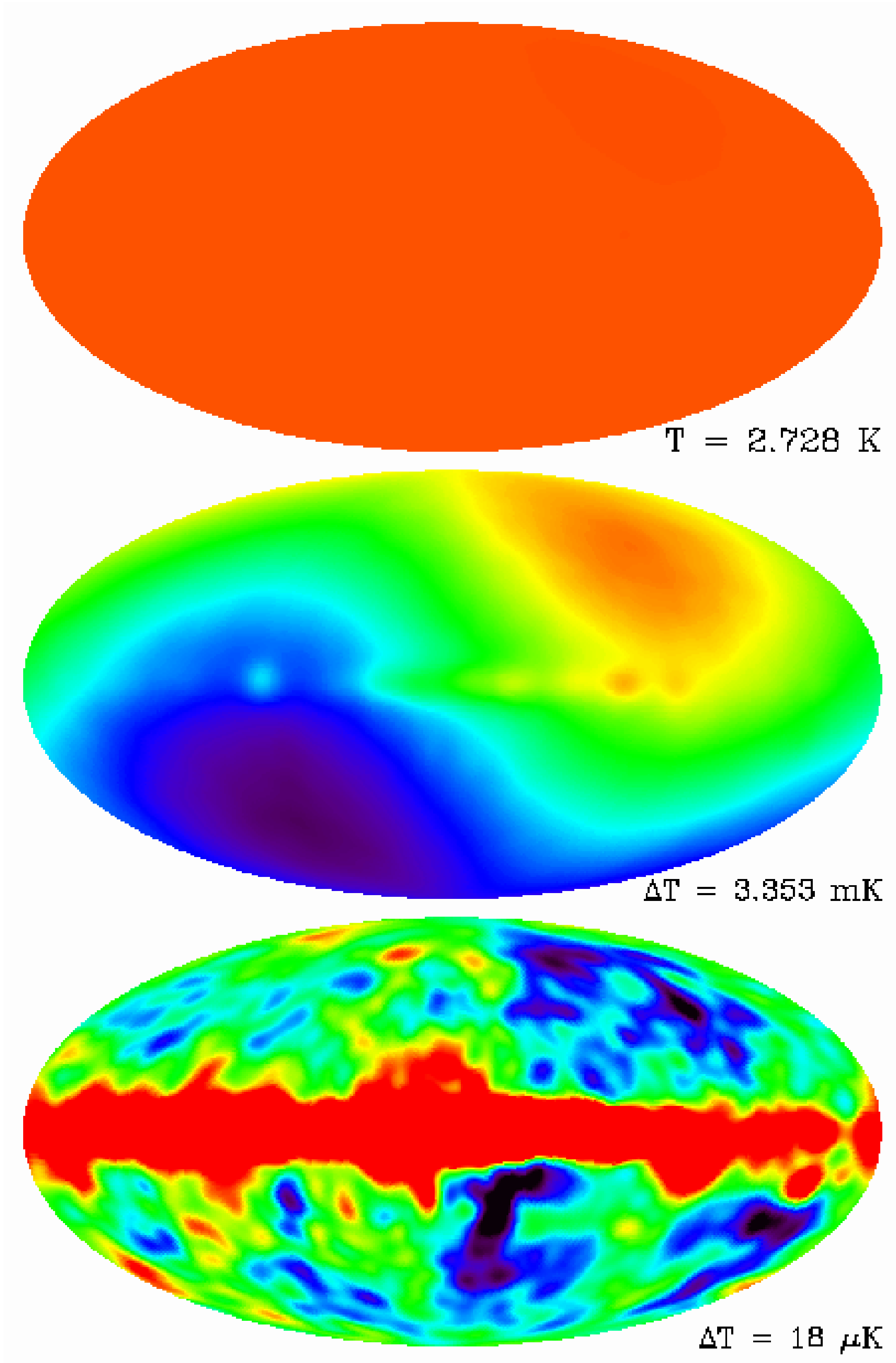

Figure 2.6: The Nobel for COBE for this

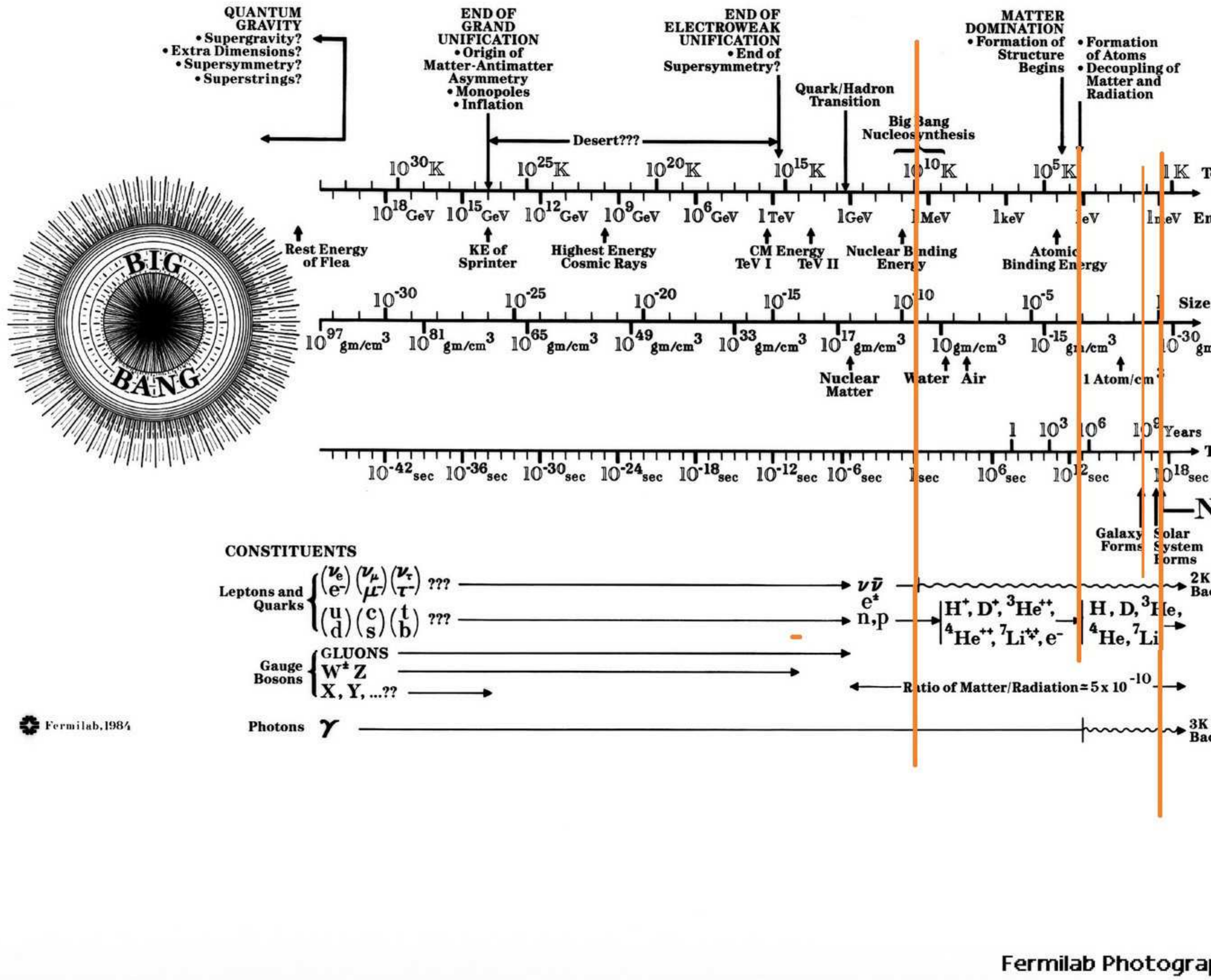

Figure 2.7: Chronology of the Big Bang

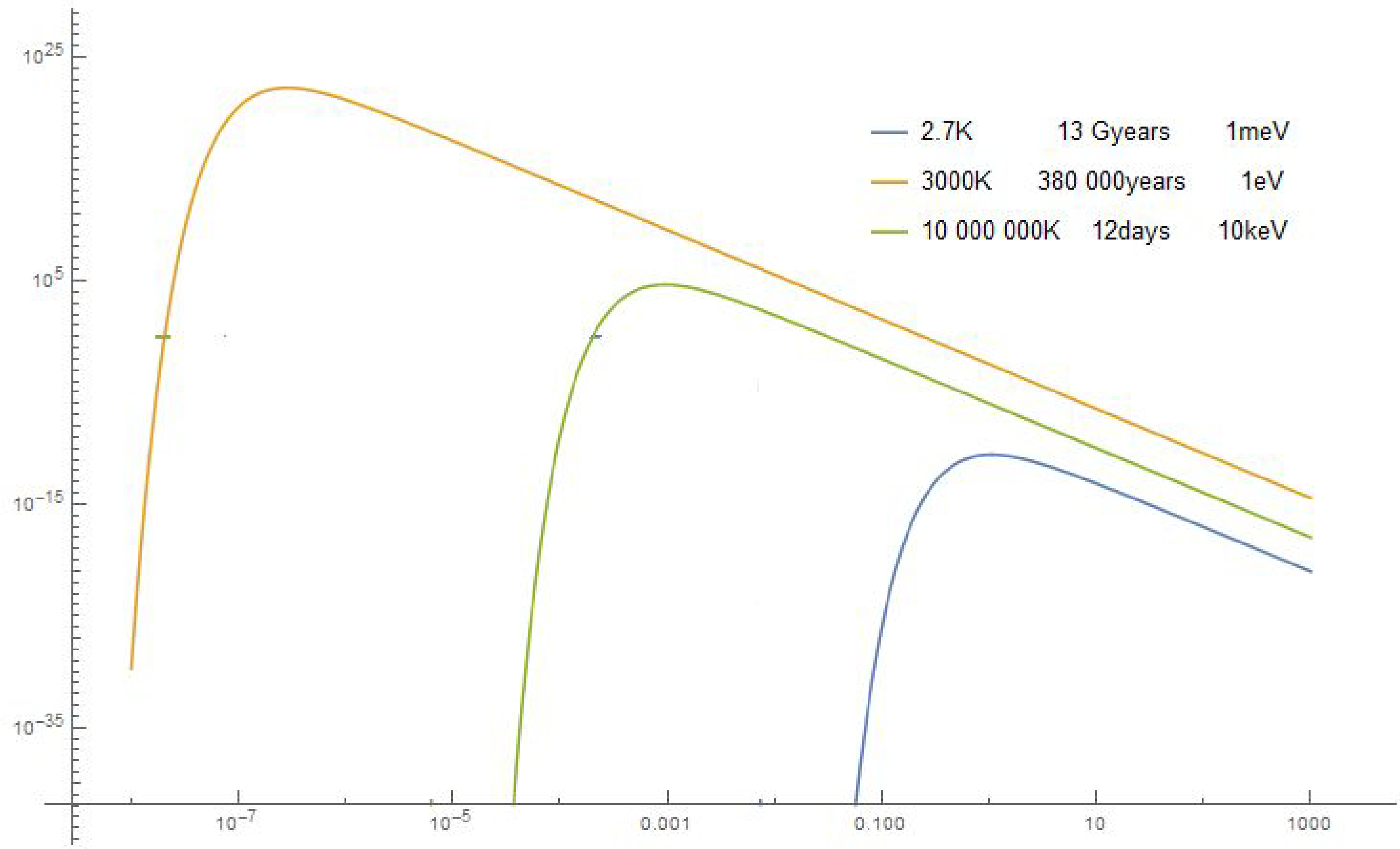

Figure 2.8: Planck spectra for three temperatures. Horizontal scale is CMBR wavelength in mm; note the absolute vertical scale! The legends give Temp of CMBR, time since BB and energy of the CMBR

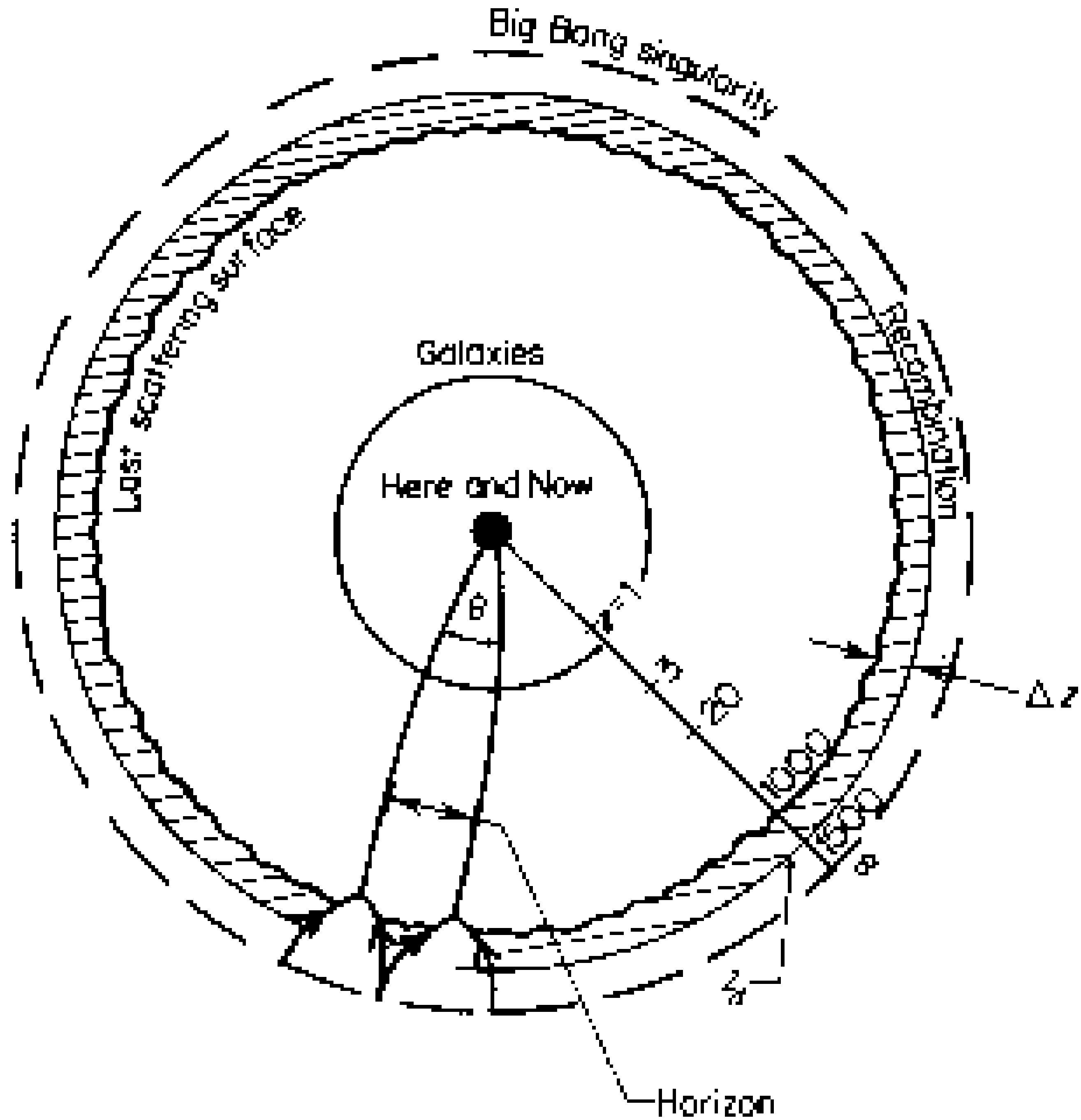

Figure 2.9: Cartoon of the surface of last scattering

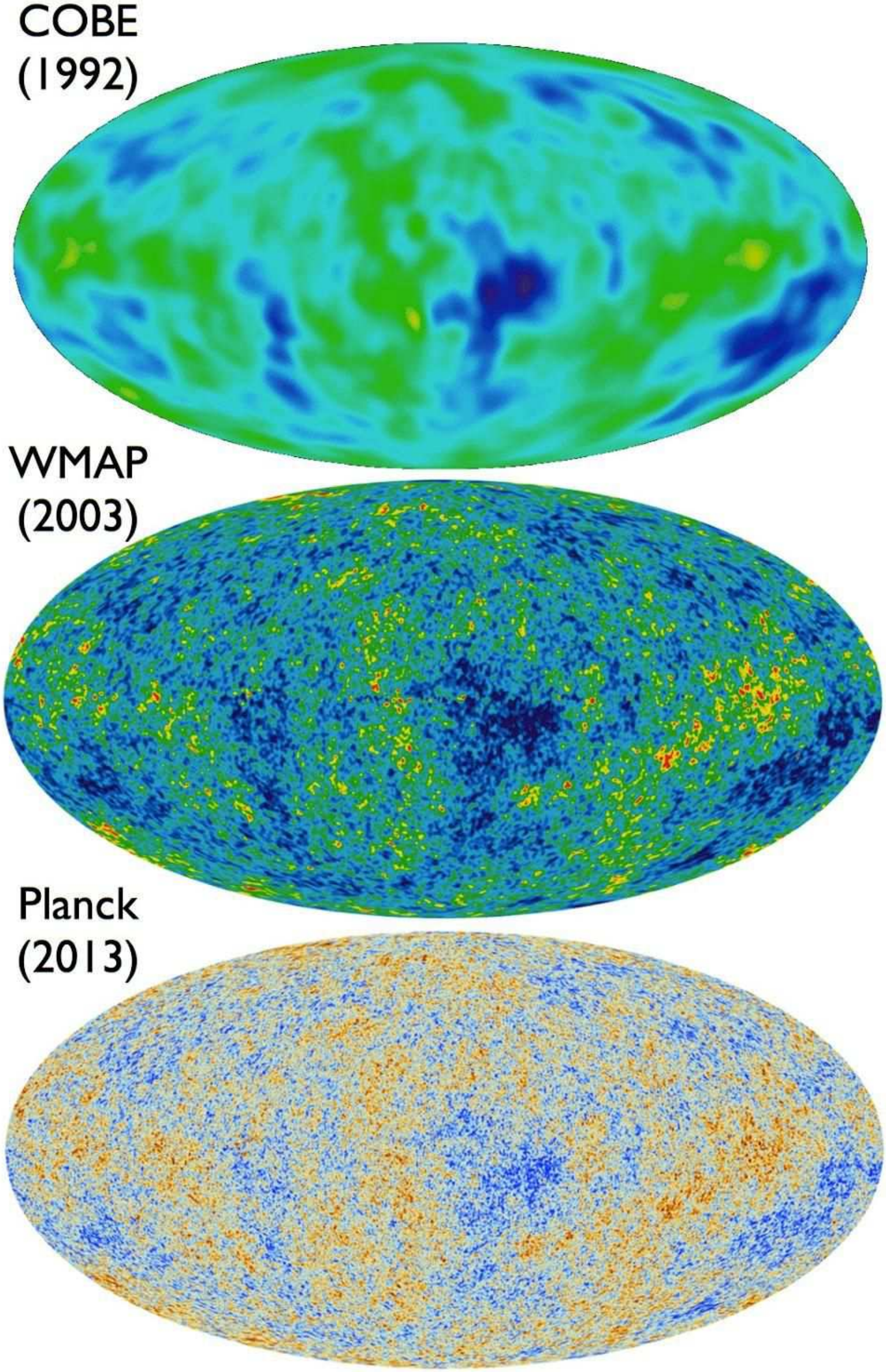

Figure 2.10: The three spacecraft experiments. COBE resolution is barely sufficient to see the first peak (see Figure 2.13); the Planck resolution cannot be improved (see Figure 2.12)

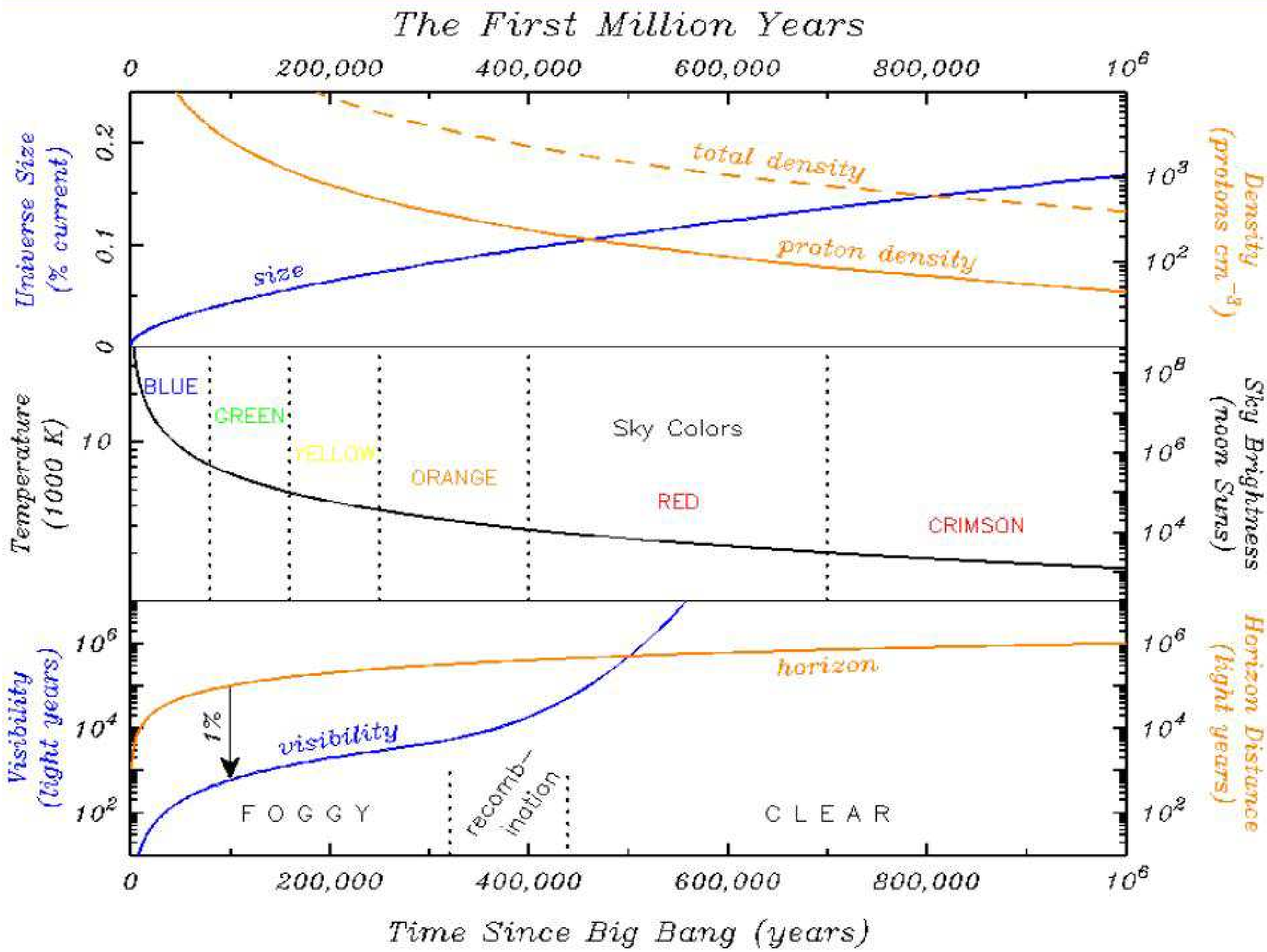

Figure 2.11: Many interesting facts about the first million years.

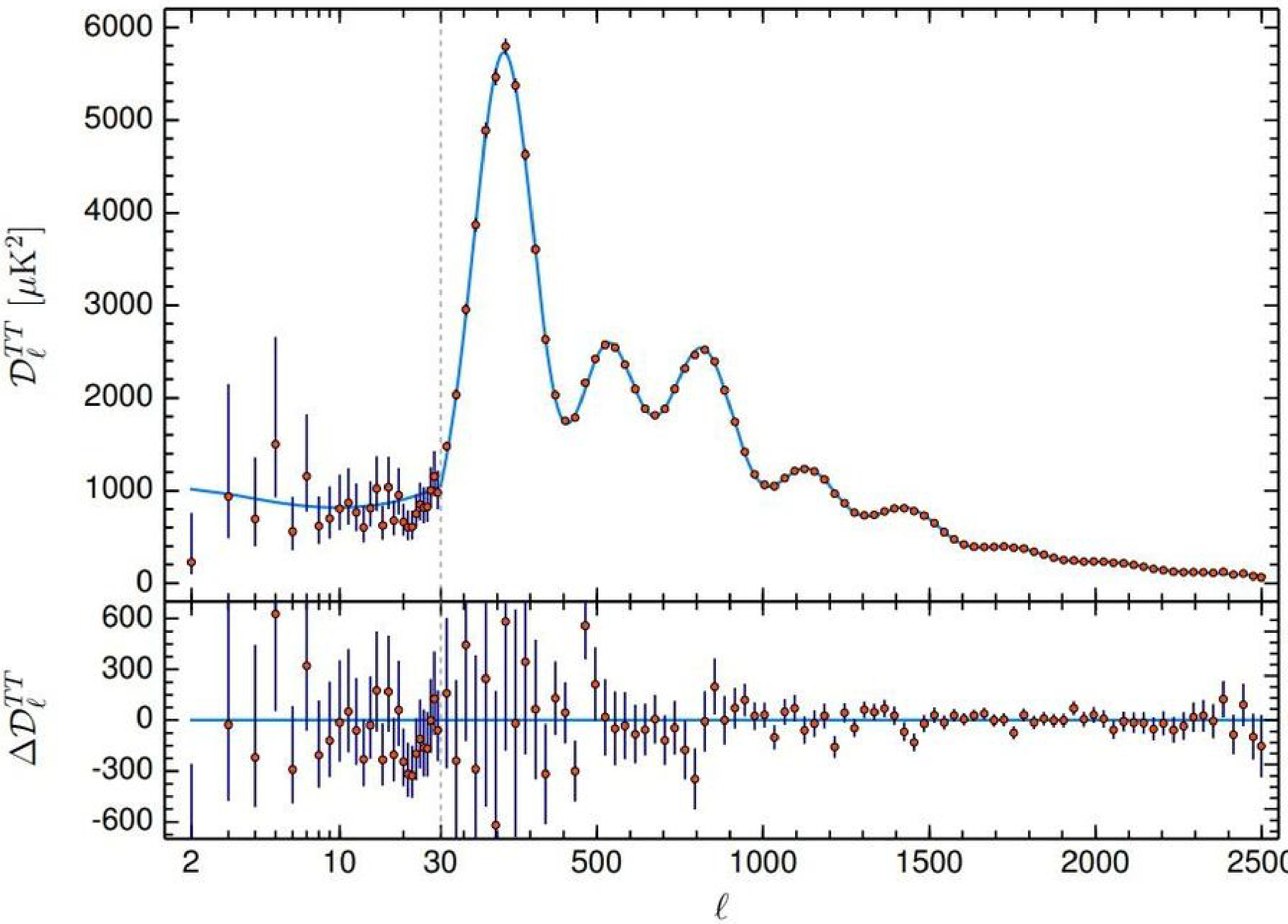

Figure 2.12: The definitive acoustic spectrum from Planck. The error bars of the residuals are multiplied by 10 on the right of the dashed like,

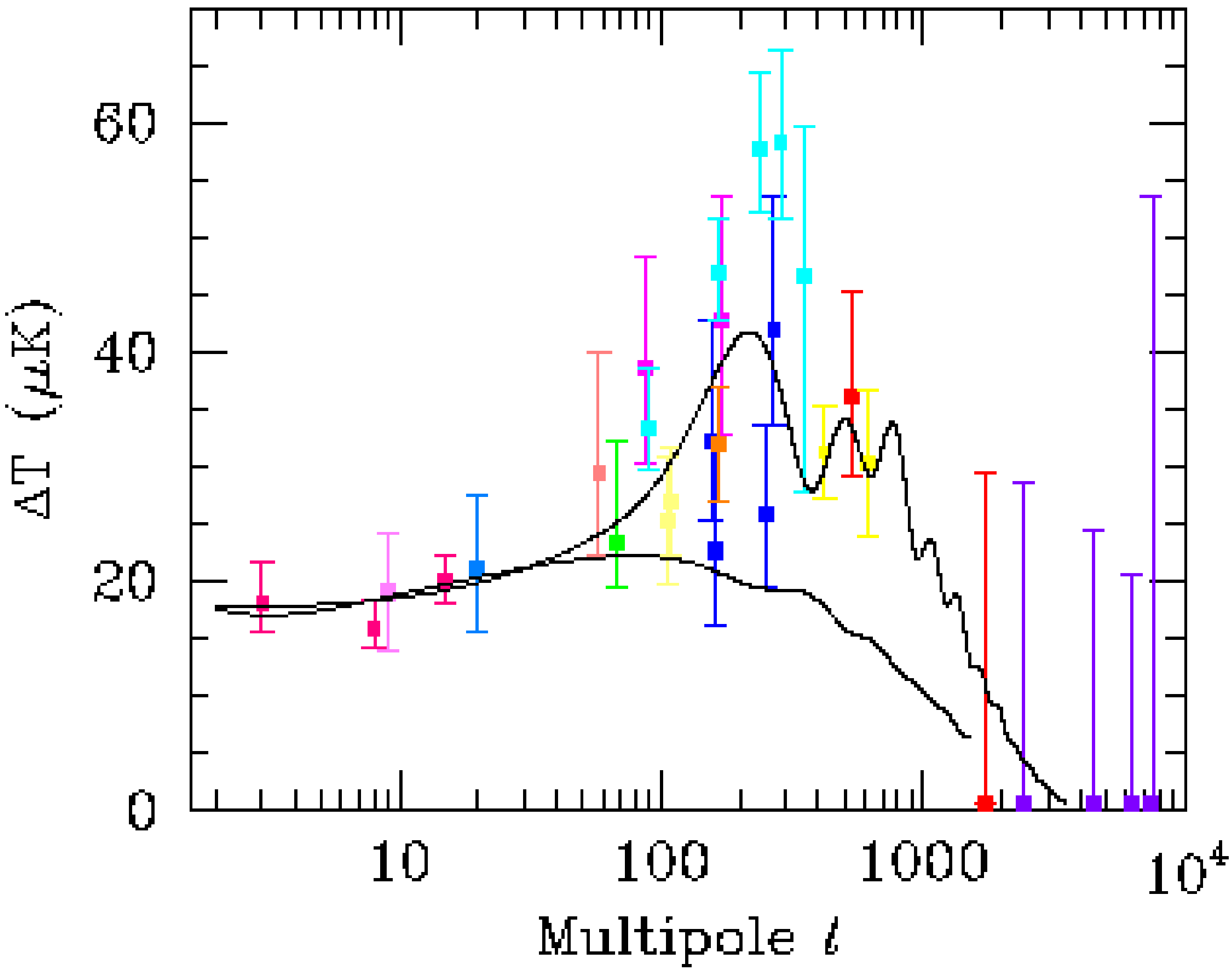

Figure 2.13: The preWMAP (i.e. also prePlanck) spectrum from 1999. The solid line is the prediction they call "the standard model". Compare with the previous plot. Those theorists in 1999 were clairvoyant(s)!!!(see text on the bottom of p.6)

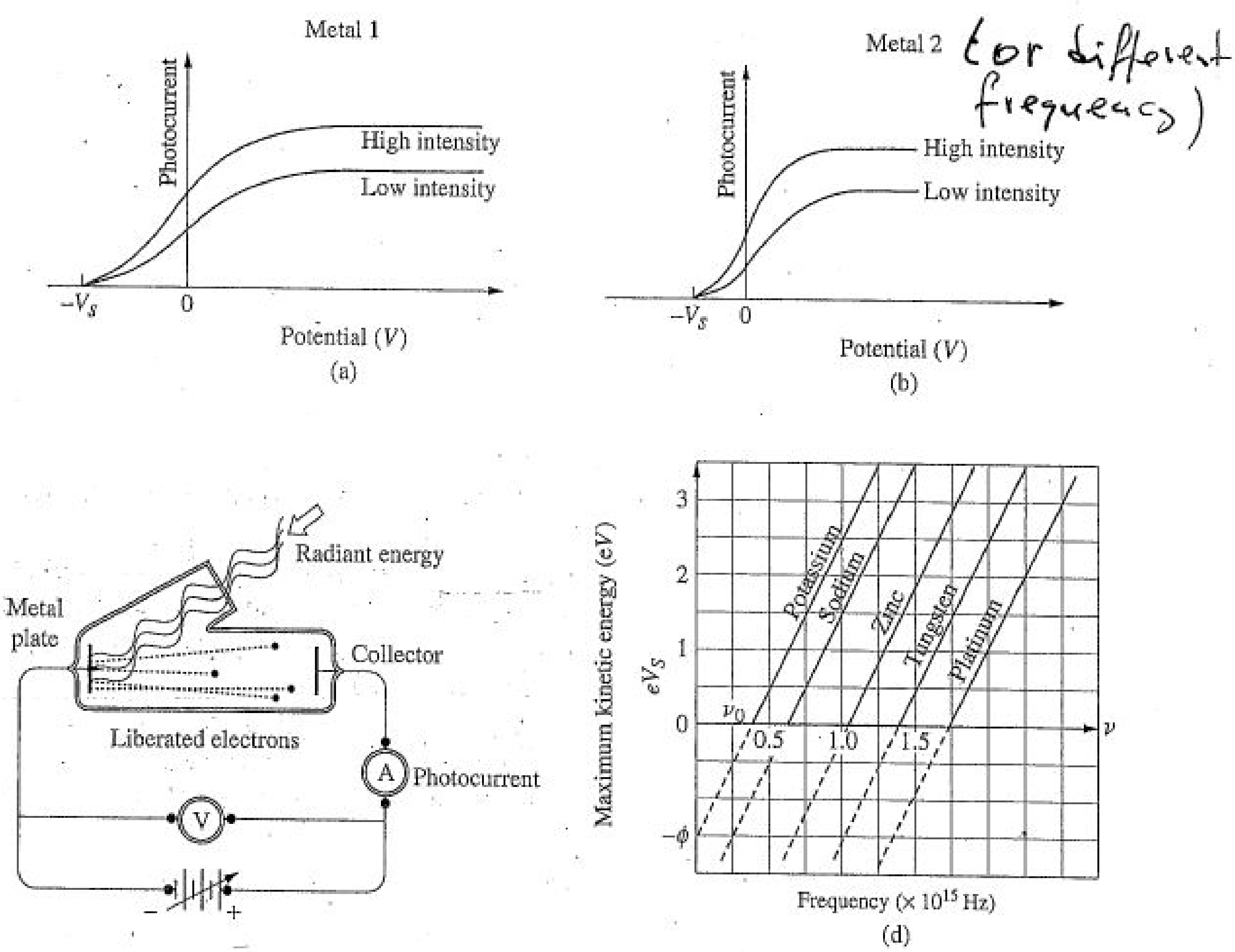

Figure 2.14: Caption for PhotoeffectCombo

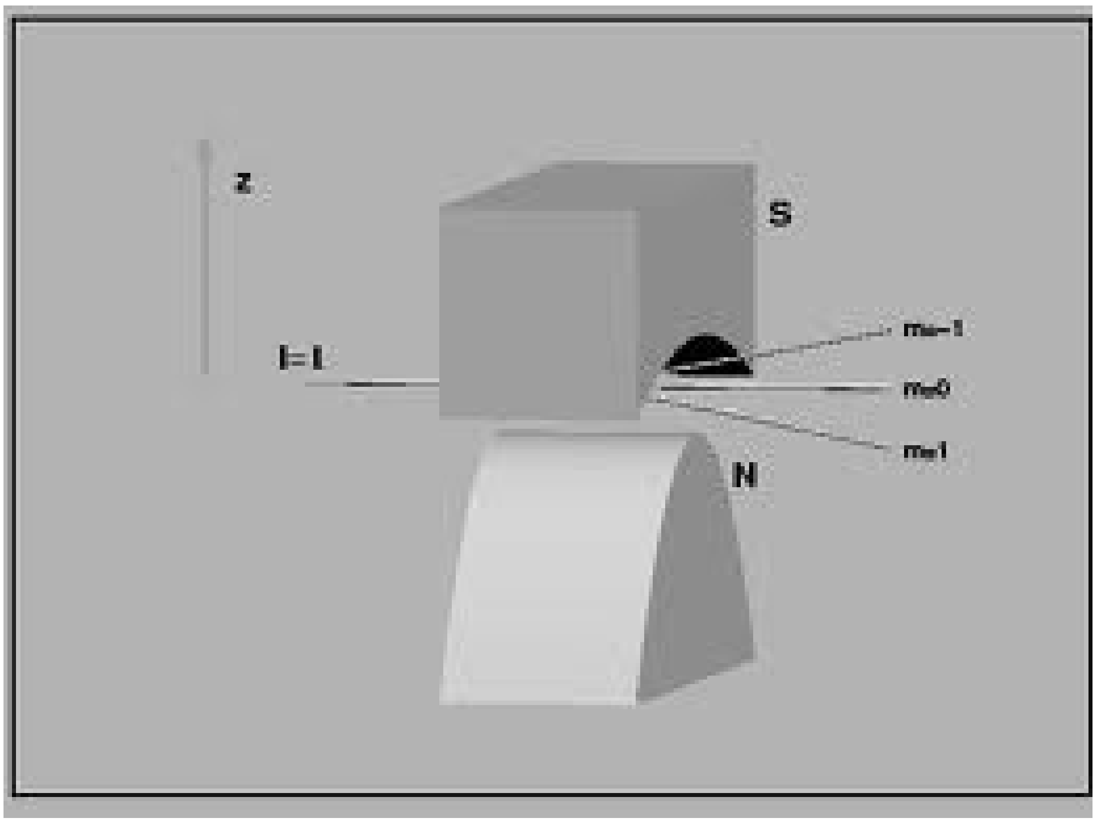

Figure 2.15: Caption for SternGerlach

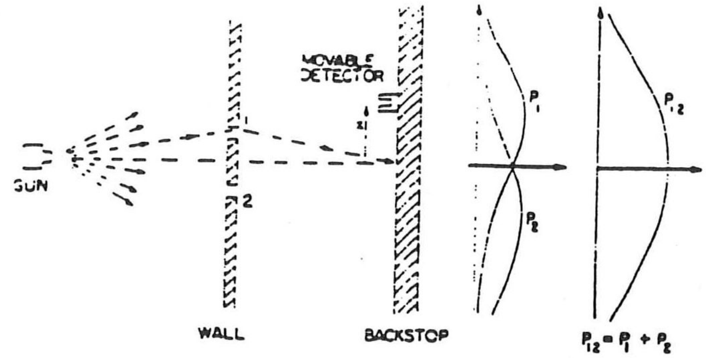

Fig. 1–1. Interference experiment with bullets.

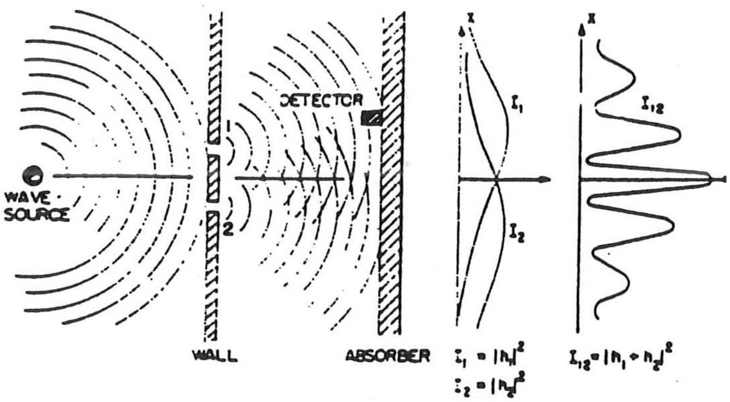

Fig. 1–2. Interference experiment with water waves.

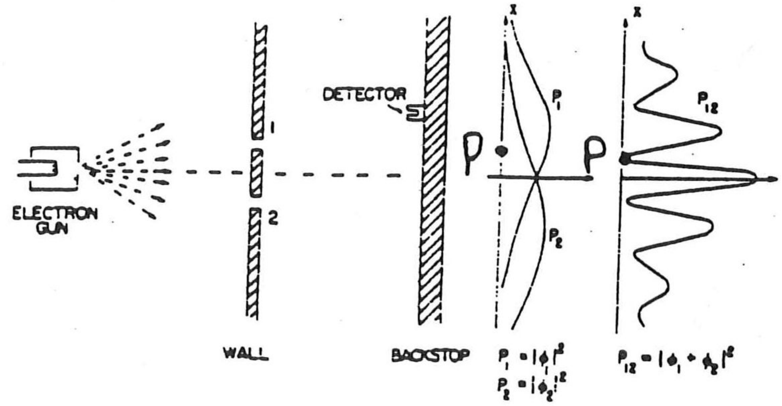

Fig. 1–3. Interference experiment with electrons.

Figure 2.16: Caption for FeynmanCentralMystery

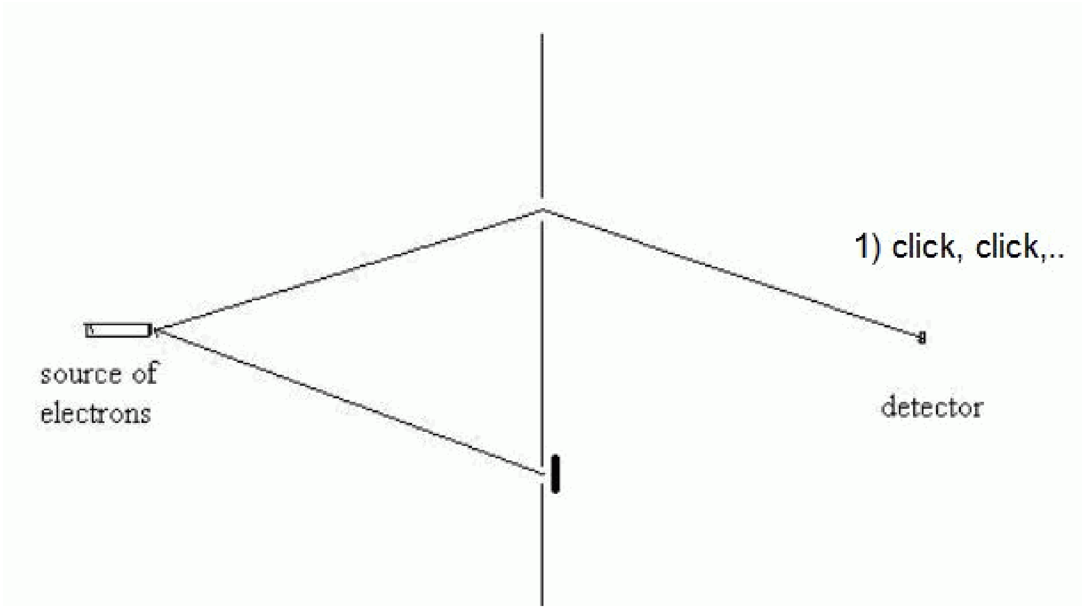

Figure 2.17: The double slit setup with the lower slit blocked; the detector is placed at the point P on Figure 2.16. You hear clicks as electron arrive at the detector.

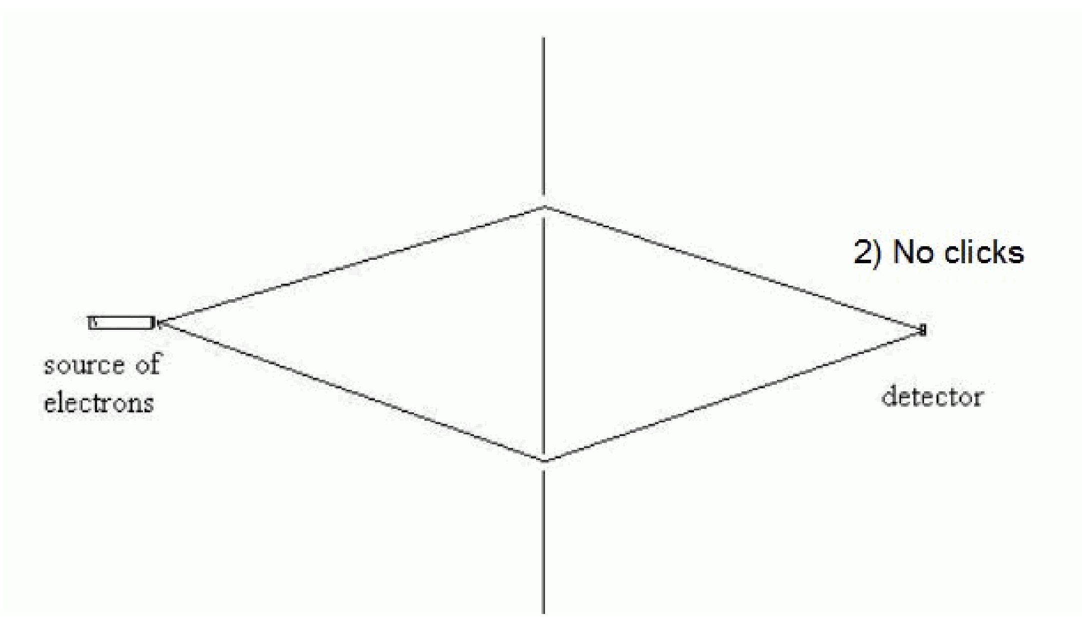

Figure 2.18: You OPEN previously closed slit, and the electrons STOP arriving

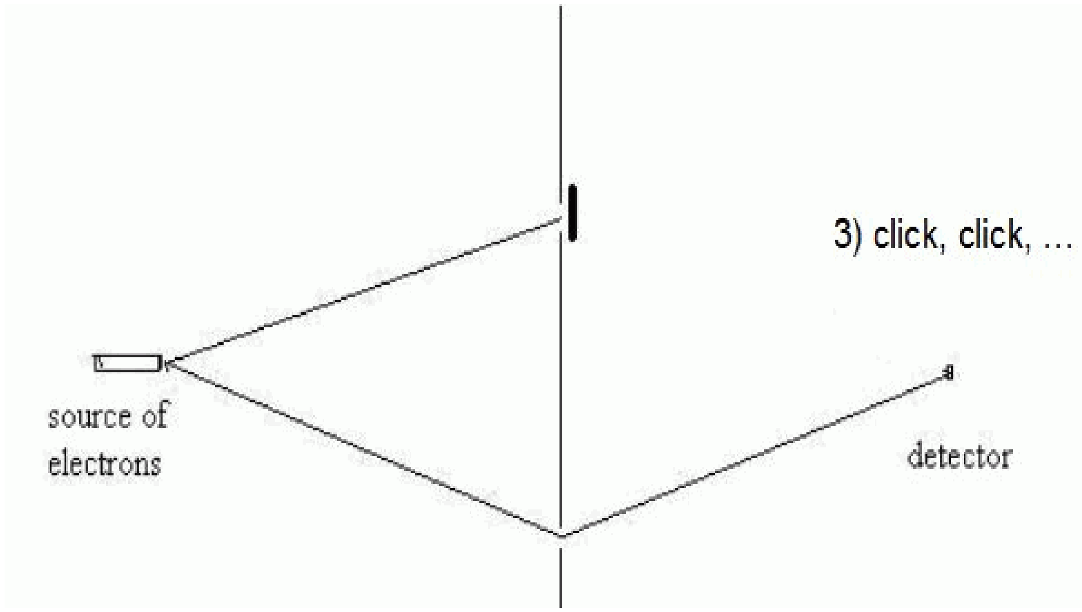

Figure 2.19: Now you close the top slit, and electrons are arriving again - click, click clikclik ...

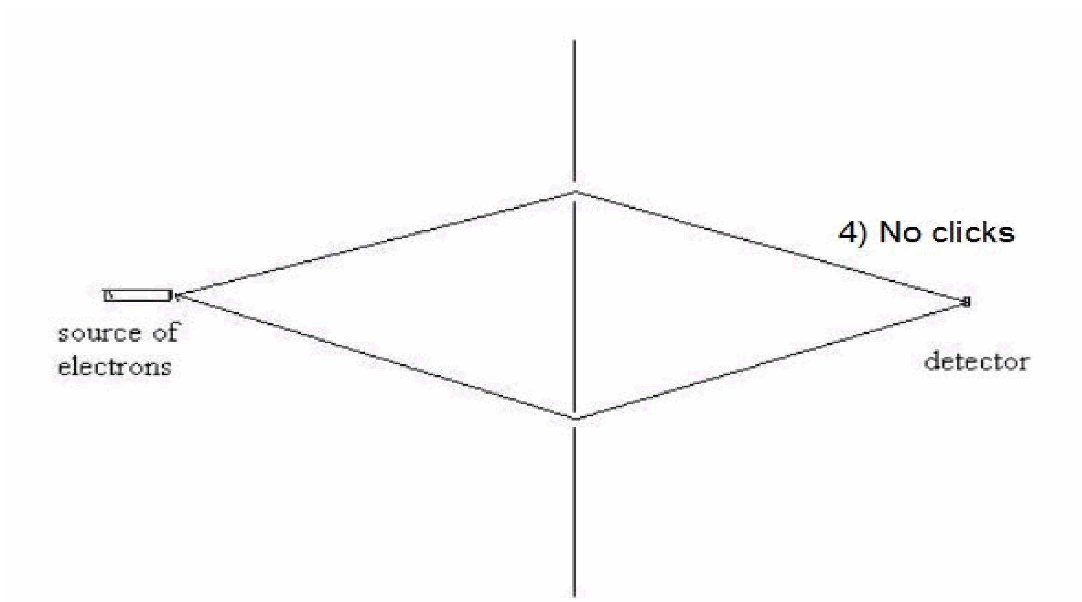

Figure 2.20: and the stop again when they have TWO paths open instead of just one ...

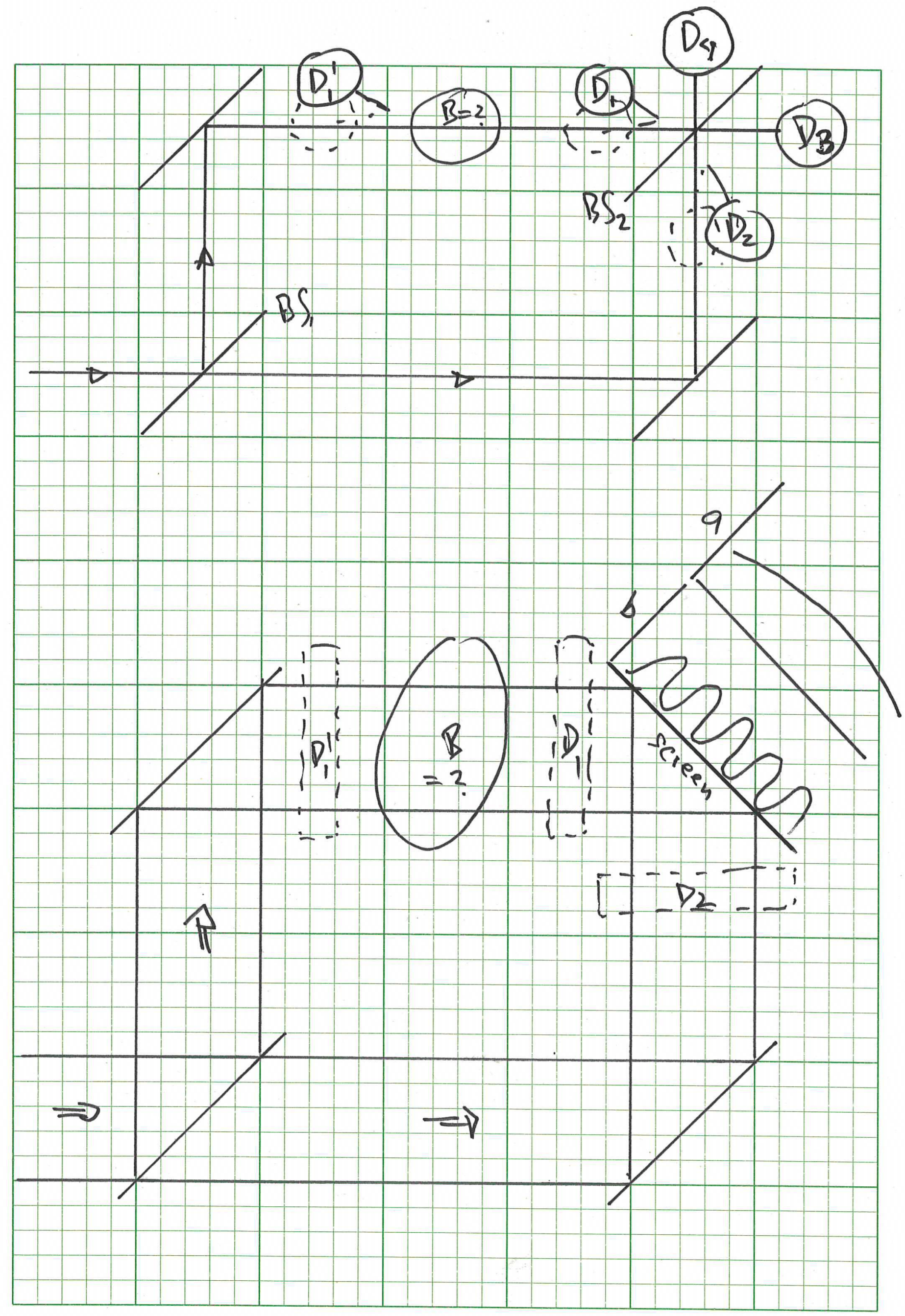

Figure 2.21: When any one of the three detectors (D_1, D_2 and D_1') is placed in the beam, the screen shows a broad, featureless signal as illustrated on a). When all three detectors are moved out of the beam, the screen shows a pattern of fringes as shown on Figure 2.22. For explanation of the element marked "B=?" see the Text.

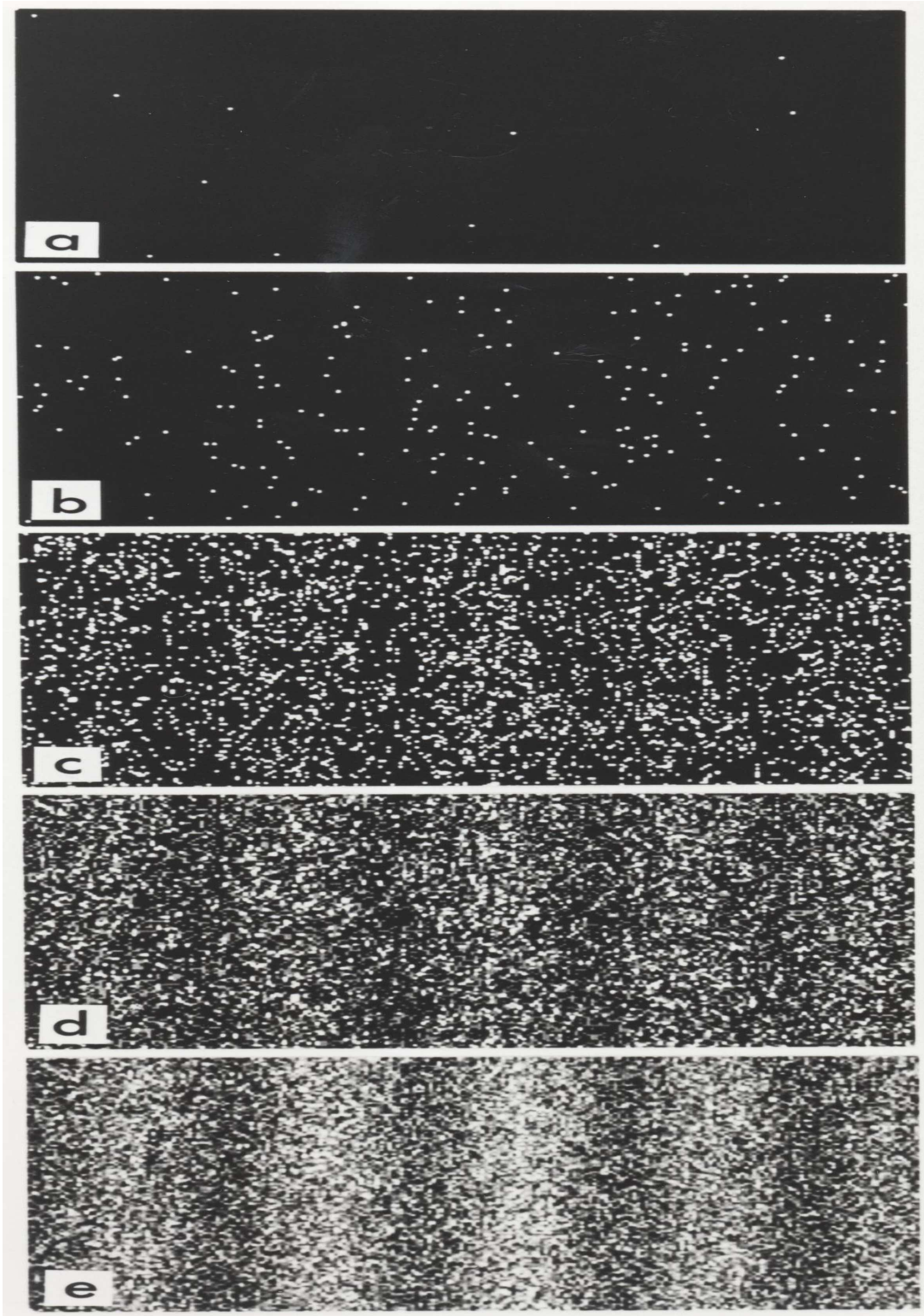

Figure 2.22: Fringes created by impacts of single particles when the two beams on Figure 2.21 are allowed to interfere. The effect persists even if the flux of particles is so low that there never is more that one particles in the spectrometer at any given time.

Chapter 3

Math I

3.1 Calculus

Familiarity with calculus is assumed. It is not a pre-requisite, since the amount of calculus needed in this course can be refreshed, or even learned from scratch, in a few days. In my experience of teaching quantum physics for many years, the math is not the problem; the real, quite difficult problem is to be able to cope with physics concept at variance with our everyday experience.

3.1.1 Differentiation

Start with a full realization that the derivative is a slope. Most rules follow from this almost immediately: derivatives of a product/ratio (HW: prove the rules from first principles); exponential and powers; function of a function; etc. You need to be able to use the l'Hospital rule (dating from 1696!) to deal with 0/0 and ∞/∞. And we will need the Taylor expansion of function $f(x)$ around the point a:

$$f(x) = \sum_{n=0}^{\infty} \frac{f^(n)(a)}{n!}(x-a)^n$$

Keeping only the first $m+1$ terms is called "working in the m-th approximation".
HW: To get a feeling for this important concept, show that in the first approximation

$$\sqrt{1+x} = 1 + x/2$$

Do this with and without the use of the Taylor expansion.

3.1.2 Integration

Integration tends to be considerably more difficult that differentiation, since we cannot apply "mechanical" rules here, and a lot of experience is needed. This course is not meant to teach you that, so for anything more complicated thn simple variable substitution, or integration by parts, we will use tables of integrals.

However, it will be very important for us to fully understand the connection between differentiation and integration, i.e. the "fundamental theorem of calculus" (HW: "prove" it from first principles"). The HW problem on the Planck discovery of the quantum is a beautiful example of this.

3.1.3 Elementary statistics:

average (mean,expectation) value: $< x >= \sum x_i P_i = \int x P(x) dx$

standard deviation ("root-mean-square"): $(\delta_x)^2 =< (x- < x >)^2 >=< x^2 > - < x >^2$

HW: in the calculation of $< E >$ for blackbody radiation, show that

from $P(E) = e^{-E/kT} \quad \Rightarrow \quad < E >= kT$

from $P_n = e^{-E_n/kT} \quad \Rightarrow \quad < E >= kT$ for low f, $< E >\rightarrow \; 0$ for high f, thus avoiding the 'ultraviolet catastrophe'. This is one of the few instances when the difference between summing and integrating is crucial ...

3.2 Complex Numbers:

The theory of the functions of complex variables is not simple, but it also is very powerful and very beautiful. (Un)fortunately, we will only need the simplest complex number concepts:

We define a complex number z

$$z = x + iy = Re(z) + i.Im(z) = a(\cos\phi + \text{i}.\sin\phi)$$

where $i^2 = -1$ - see Figure 3.1

The elementary operations with complex numbers follow immediately:

$$|z| = \sqrt{x^2 + y^2} \qquad z_1 + z_2 = (x_1 + x_2) + i(y_1 + y_2) \qquad z_1 z_2 = (x_1 x_2 - y_1 y_2) + i(x_1 y_2 + x(2y_1)$$

3.2.1 Feynman's "Amazing Jewel"

Chapter 22 of Volume I of the celebrated Feynman Lectures begins by stating:

"In our study of oscillating systems we shall have occasion to use one of the most remarkable, almost astounding, formulas in all of mathematics ... an amazing jewel ..."

I cannot resist from sharing some of my admiration for Feynman genius and wisdom, as well as his remarkable skills in manipulating numbers. So here is a simplified version of his brilliant celebration of the power of human reasoning – normally one does this proof using calculus. Feynman does it "from first principles":

Consider the function $f(x) = e^x$ where "e" is the base of the natural logarithms e=2.71828... . Using your calculator you can easily confirm, to arbitrary precision, that for very small values[1]

$$f(d) = e^d = 1 + d$$

Since any number D that is not small can be expressed as sum of many small numbers: D = d+d+d+d+....d, and since $e^{a+b} = e^a e^b$, we get

$$e^D = e^d e^d e^d ... e^d = (1 + d)(1 + d)(1 + d)...(1 + d)$$

The first three columns on Figure 3.2 show a simple EXCEL calculation demonstrating this.

Complex numbers obey all the usual rules (as long as you always substitute $i^2 = -1$).So assume that the above equation is also true for $d = i\phi$ where ϕ is very small. Then for $D = i\Phi$ when Φ is not small, we can follow the above logic, split Φ into N pieces all equal to $\phi = \Phi/N$ and we get

$$e^{i\Phi} = e^{i\phi} e^{i\phi} e^{i\phi} ... e^{i\phi} = (1 + i\phi)(1 + i\phi)(1 + i\phi)...(1 + i\phi)$$

and we can easily evaluate this for any value of the argument Φ (again, always remembering that $i^2 = -1$). The results of the corresponding EXCEL calculation is on Figure 3.2, and you can check, to arbitrary precision, that the real part is nothing but $\cos\Phi$ and imaginary part is $\sin\Phi$, so that

$$e^{i\Phi} = \cos\Phi + i\sin\Phi$$

for any value of Φ (see the top of Figure 3.3) .

This is the promised equation (usually called the **Euler formula**): spectacular from many points of view, and ubiquitous in mathematics, physics, signal processing and just about any branch of the "hard" sciences.

3.2.2 Some applications of the Euler formula

Previously, we used the "Cartesian" representation $z = x + iy$. The Euler formula provides the "polar" representation

$$z = ae^{i\phi}$$

As we saw above, the Cartesian form is useful for linear operations (e.g. $z_1 + z_2 = (x_1 + x_2) + i(y_1 + y_2)$ etc.).

The Euler formula implies

$$z_1 z_2 = a_1 a_2 e^i \phi 1 + \phi 2 \qquad z_1/z_2 = \frac{a_1}{a_2} e^{i(\phi_1 - \phi_2}$$

This makes the polar form useful for multiplication, division and exponentiation (e.g. $z_1/z_2 = (a_1/a_2)e^{i(\phi_1-\phi_2)}$, $\sqrt{z} = \sqrt{a}e^{i\phi/2}$ etc.).
Notes:

[1] Hint: start by using $d = 0.1$ and you will get $e^d = 1.105...$. This differs from $1 + d$ just by 0.5% - good but not good enough for our use. So try d=0.01, 0.001, 0.0001 and see what happens).

1. A very useful expression that immediately follows is $i = e^{i\pi/2}$. That can be used to determine, for example

$$\sqrt{i} = \sqrt{e^{i\pi/2}} = (e^{i\pi/2})^{1/2} = e^{i\pi/4} = (1+i)/\sqrt{2}$$

2. Even more fun is

$$i^i = (e^{i\pi/2})^i = e^{-\pi/2}$$

which means that

$$i^i e^{\pi/2} - 1 = 0$$

Just about all mathematical symbols, some seemingly not related, are connected in this single expression[2]!

3. A less fanciful but much more useful example is a trigonometric application:

$$e^{i(\alpha\pm\beta)} = \cos(\alpha\pm\beta) + i\sin(\alpha\pm\beta) = e^{i\alpha}e^{i\beta} = (\cos\alpha \pm i\sin\alpha)(\cos\beta \pm i\sin\beta)$$

Equating the both sides of the real and imaginary parts of the second expression with those of the 4th expression, you get some very useful trigonometric formulas. Just try to prove them without complex numbers (the way the ancients did it :-)

4. complex conjugation:

$$z^* = x - iy = ae^{-i\phi} \qquad |z| = \sqrt{z.z^*} = a = \sqrt{x^2+y^2}$$

5. Note the origin of the Euler formula in the expansion

$$e^b = 1 + b + b^2/2! + b^3/3! + b^4/4! + b^5/5! + ...$$

for $b = i\phi$.

HW: Determine real and imaginary part of $\sqrt{i}$, i^i (proving the remarkable equation $i^i e^{\pi/2} - 1 = 0$), and derive the expressions for $sin(\alpha+\beta)$ and $\cos(\alpha+\beta)$

3.3 The Dirac Delta function

Consider a limiting process in which a function which peaks at a given position (say at x=a) gets narrower and narrower while keeping its integral (i.e. the area beneath the graph) equal to 1 - see 3.5. In the limit, this becomes a remarkable "function" $\delta(x-a)$ which is equal zero everywhere except at x=a, and yet

$$\int f(x)\delta(x-a)dx = f(a)$$

[2] We should note that our expression is just one of infinitely many that follow from the fact that the $\sqrt{-1}$ can also be written as $i = -e^{i2\pi/2}$, $i = e^{i3\pi/2}$, $i = -e^{i4\pi/2}$ etc.

for arbitrary function $f(x)$ - see Figure Mathematicians call such a creature a "distribution" or a "functional", but we will call it the "Dirac delta-function" - it is ubiquitous in many Physics applications.
The delta function is the limit of various peaked functions - some of the many possible 'representations' are graphical **??**, some are analytical. For our use, the most useful analytical form will be

$$\delta(x) = (1/2\pi) \int_{-\infty}^{\infty} e^{ikx} dk = 1/2\pi) \lim_{L\to\infty} \int_{-L}^{L} e^{ikx} dk \sim \lim_{L\to\infty} L \frac{\sin Lx}{Lx}$$

HW: fill-in the missing steps (hint: see Figure 3.4) **Notes:**

the Dirac δ function is not square-integrable:

$$\int \delta(x) dx = 1 \quad \text{but} \quad \int \delta^2(x) dx = \delta(0) = \infty \; !$$

The resulting normalization problems, when not trivial, are resolved by using wave packets, or by using a box-normalization with large but finite L.

In order to fully appreciate the defining property of the δ function:

$$\int f(x) \delta(x-y) dx = f(y)$$

it is useful to compare it with the analogous property of the discrete case:

$$\sum_n f_n \delta_{nk} = f_k$$

with the Kronecker delta defined as $\delta_{mn} = 0$ for $m \neq n$, $\delta_{mm} = 1$.

Many other properties of the delta-function are easily demonstrated using the behavior of the defining integral.

3.3.1 The Fourier Transform

Define

$$F(k) = (1/\sqrt{2\pi}) \int f(x) e^{-ikx} dx$$

Then it is easy, using our (newly acquired, maybe) knowledge of the δ-function, to see that

$$(1/\sqrt{2\pi}) \int F(k) e^{ikx} dk = f(x)$$

(In order to acquire not just the knowledge but also some degree of familiarity, it is very useful to prove this (hint: just take $F(k)$ from the second equation and plug it into the first equation. There is subtlety in there that is very important for you to understand).

These two expressions form the famous Fourier transform and its inverse (if you had QM previously you are probably more familiar with Fourier transform with variables (x,p) instead of (t,ω) - the latter is important in Acoustics but it is exactly the same thing ...).

3.3.2 The Fourier Series

When the "spectrum" $F(k)$ happens to be a sum of discrete, equidistant peaks:

$$F(k) = \sum_{-\infty}^{\infty} \sqrt{2\pi} a_n \delta(k - nk_1)$$

it is easy to see that the resulting $f(x)$ will be periodic with period $2L = 2\pi/k_1$, described by a Fourier series:

$$f(x) = \sum_{n=0}^{\infty} A_n \cos\frac{n\pi x}{L} + \sum_{n=1}^{\infty} B_n \sin\frac{n\pi x}{L} = \sum_{-\infty}^{+\infty} a_n e^{in\pi x/L}$$

We see that Fourier series is a special case of Fourier transform (and remarkably, also in the opposite direction: any periodic function can be shown to have spectrum consisting of equidistantly-spaced delta-functions ...).

The 'base' functions $e^{in\pi x}$ satisfy an obvious (and very useful) **orthonormality** condition:

$$\frac{1}{2L} \int_{-L}^{+L} e^{in\pi x/L} e^{-im\pi x/L} = \delta_{mn}$$

This enables a determination of the coefficients: multiplying the expansion of $f(x)$ by $e^{-im\pi x/L}$, and integrating over x, one gets

$$a_m = \frac{1}{2L} \int_{-L}^{+L} f(x) e^{-im\pi x/L}$$

Remarkably (again :-) we can also show that Fourier transform is a special case of Fourier series:

Define

$$k = \pi n/L \qquad F(k) = \sqrt{\frac{2}{\pi}} L a_n$$

and make transition $L \to \infty$ (i.e. $\Delta k = \pi/L \to dk$, and replace the sum by an integral):

$$f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} F(k) e^{ikx} dk$$

The inverse transform follows from the expression for a_n:

$$F(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} f(x) e^{-ikx} dx$$

For a simple illustration of the Fourier Transform see Figure **??**. We will see many illustrations, applications and generalizations of Fourier in this course.

3.4 Figures

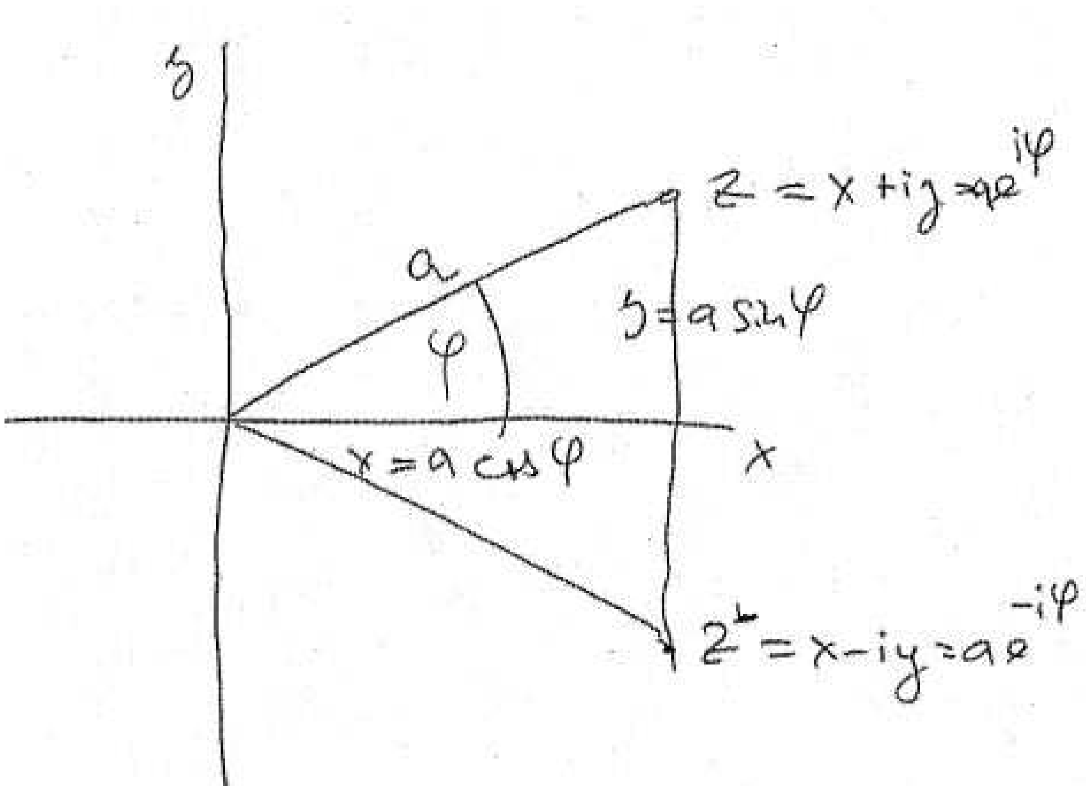

Figure 3.1: Graphical representation of numbers in the “complex plane”.

	A	B	C	D	E	F	G	H	I	J
1	x	e^x estim	e^x		phi	degrees	Im	sin	Re	cos
2	0	1	1		0	0	0	0	1	1
3	5E-05	1.00005	1.0001		0.0001	0.0073	0.0001	0.0001	1	1
4	0.0001	1.0001	1.0001		0.0003	0.0146	0.0003	0.0003	1	1
5	0.0002	1.0002	1.0002		0.0005	0.0293	0.0005	0.0005	1	1
6	0.0004	1.0004	1.0004		0.001	0.0586	0.001	0.001	1	1
7	0.0008	1.0008	1.0008		0.002	0.1172	0.002	0.002	1	1
8	0.0016	1.0016	1.0016		0.0041	0.2344	0.0041	0.0041	1	1
9	0.0032	1.00321	1.0032		0.0082	0.4688	0.0082	0.0082	1	1
10	0.0064	1.00642	1.0064		0.0164	0.9375	0.0164	0.0164	0.9999	0.9999
11	0.0128	1.01288	1.0129		0.0327	1.875	0.0327	0.0327	0.9995	0.9995
12	0.0256	1.02593	1.0259		0.0654	3.75	0.0654	0.0654	0.9979	0.9979
13	0.0512	1.05253	1.0525		0.1309	7.5	0.1305	0.1305	0.9915	0.9914
14	0.1024	1.10782	1.1078		0.2618	15	0.2588	0.2588	0.9659	0.9659
15	0.2048	1.22727	1.2273		0.5236	30	0.5	0.5	0.8661	0.866
16	0.3072	1.3596	1.3596		0.7854	45	0.7071	0.7071	0.7071	0.7071
17	0.4096	1.5062	1.5062		1.0472	60	0.8661	0.866	0.5	0.5
18	0.512	1.6686	1.6686		1.309	75	0.966	0.9659	0.2588	0.2588
19	0.6144	1.84852	1.8485		1.5708	90	1.0001	1	9E-09	3E-16
20	0.7168	2.04783	2.0479		1.8326	105	0.966	0.9659	-0.2588	-0.2588
21	0.8192	2.26864	2.2687		2.0944	120	0.8661	0.866	-0.5001	-0.5
22	0.9216	2.51325	2.5133		2.3562	135	0.7072	0.7071	-0.7072	-0.7071
23	1.024	2.78424	2.7843		2.618	150	0.5001	0.5	-0.8662	-0.866
24	1.1264	3.08445	3.0845		2.8798	165	0.2589	0.2588	-0.9661	-0.9659
25	1.2288	3.41702	3.4171		3.1416	180	2E-08	-3E-16	-1.0002	-1
26	1.3312	3.78546	3.7856		3.4034	195	-0.259	-0.259	-0.9661	-0.9659
27	1.4336	4.19362	4.1938		3.6652	210	-0.5	-0.5	-0.8662	-0.866
28	1.536	4.64579	4.646		3.927	225	-0.707	-0.707	-0.7073	-0.7071
29	1.6384	5.14672	5.1469		4.1888	240	-0.866	-0.866	-0.5001	-0.5
30	1.7408	5.70165	5.7019		4.4506	255	-0.966	-0.966	-0.2589	-0.2588
31	1.8432	6.31643	6.3167		4.7124	270	-1	-1	-3E-08	-2E-16
32	1.9456	6.99749	6.9978		4.9742	285	-0.966	-0.966	0.2589	0.2588
33	2.048	7.75198	7.7524		5.236	300	-0.866	-0.866	0.5002	0.5
34	2.1504	8.58783	8.5883		5.4978	315	-0.707	-0.707	0.7074	0.7071
35	2.2528	9.5138	9.5143		5.7596	330	-0.5	-0.5	0.8663	0.866
36	2.3552	10.5396	10.54		6.0214	345	-0.259	-0.259	0.9663	0.9659
37	2.4576	11.676	11.677		6.2832	360	-3E-08	-2E-15	1.0004	1

Figure 3.2: Feynman's Jewel: $e^{i\Phi} = \cos\Phi + i\sin\Phi$

First check that the procedure works for e^x with a *real* exponent: the first three columns show the values of x (A), the results of the iterative procedure as calculated (B), compared with the values of e^x from my calculator (C). The procedure does work. Showing more decimal places would show small differences (that would be cured by dividing x into even smaller pieces, and so on).

Now apply the procedure on $e^{i\Phi}$.
The first two columns are:
the angle Φ in Radians (E) and degrees (F)
next 2 columns: Imaginary part of $e^{i\Phi}$ as calculated (G), compared to $\sin\Phi$ from the calculator (H);
next 2 columns: Real part of $e^{i\Phi}$ as calculated (I) and compared to $\cos\Phi$ (J)

So we see that indeed $e^{i\Phi} = \cos\Phi + i\sin\Phi$

Technical "detail": Following Feynman's clever way of dealing with the rounding errors, we first proceed by doubling the argument (the first 14 rows) then switch to increasing the argument linearly (by 0.1024 Radians for e^x and by 15 degrees for $e^{i\Phi}$).

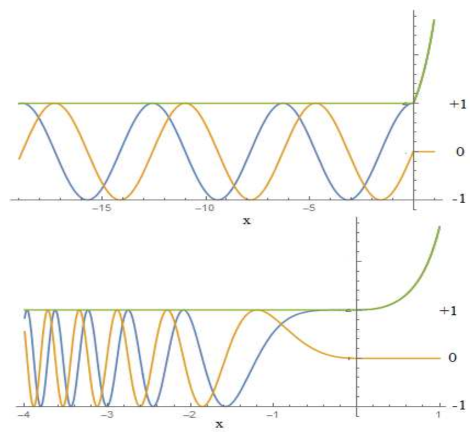

Figure 3.3: Top: (Wolfram) Mathematica plot of the function $f_0(x) = e^{xSqrt(Sign(x))}$ blue=Re(f_0), yellow = Im(f_0) and green is the magnitude $\sqrt{Re^2 + Im^2}$
Bottom: The above function $f_0(x)$ correctly depicts the sine and cosine for left-hand (imaginary) side adding to a constant magnitude, and the purely real exponential on the right-hand side. It is continuous at x=0 but the derivative is not – after all, it corresponds to an abrupt change of direction from descending along the real axis to increasing along the perpendicular imaginary axis. Also, it is not a "genuine" function but a "trick" to combine two functions together. One elegant way to improve the illustration is to plot for example the function $f_5(x) = e^{x^{5/2}}$ shown here – the transition between oscillatory and exponential behavior is smooth. It is fun to see how the functions $f_3, f_5, f_7...$ evolve. And it is a nice little exercise in calculus to see why the simplest choice $f_1(x) = e^{x^{1/2}}$ does not work.

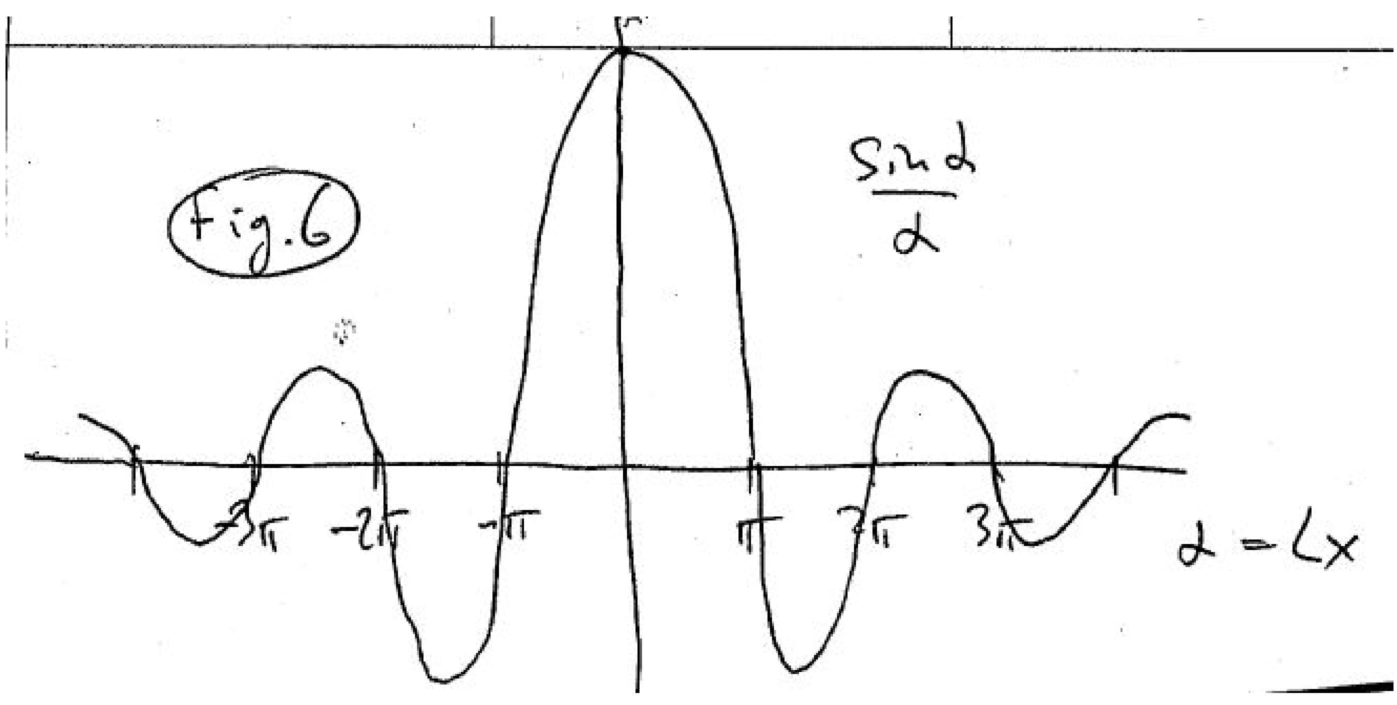

Figure 3.4: What happens when a) $\alpha \to \infty$ b) $L \to \infty$?

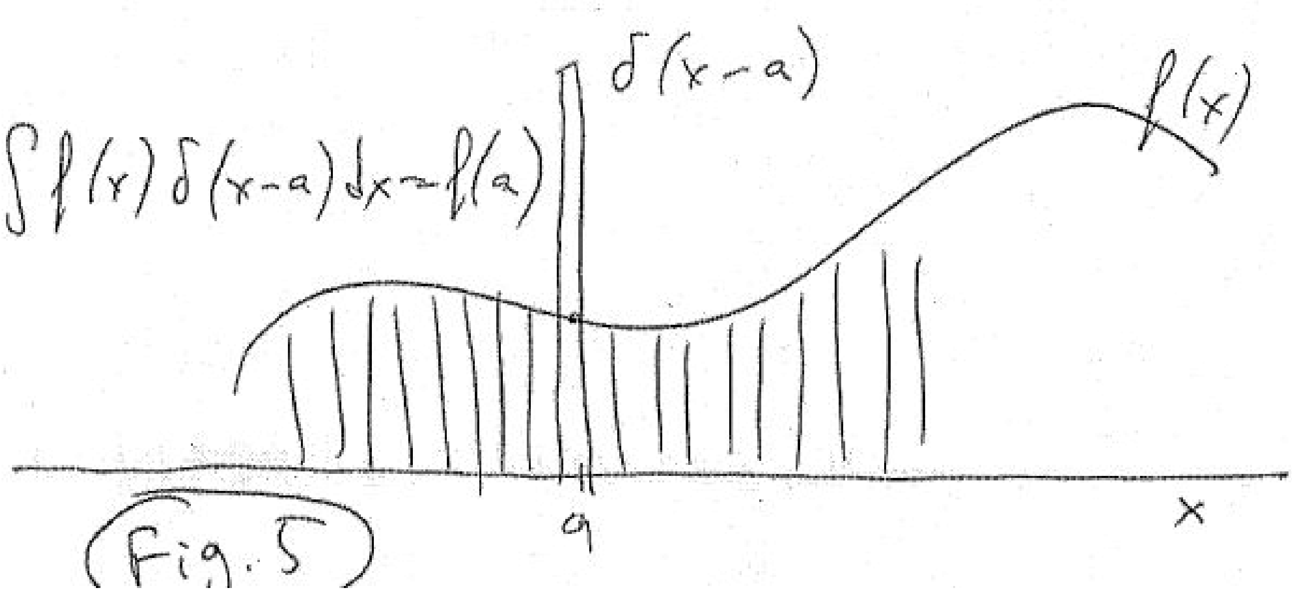

Figure 3.5: In order to better understand the defining property of the δ function: $\int f(x)\delta(x-y)dx = f(y)$ it is useful to compare it with the analogous property of the discrete case: $\sum_n f_n \delta_{nk} = f_k$

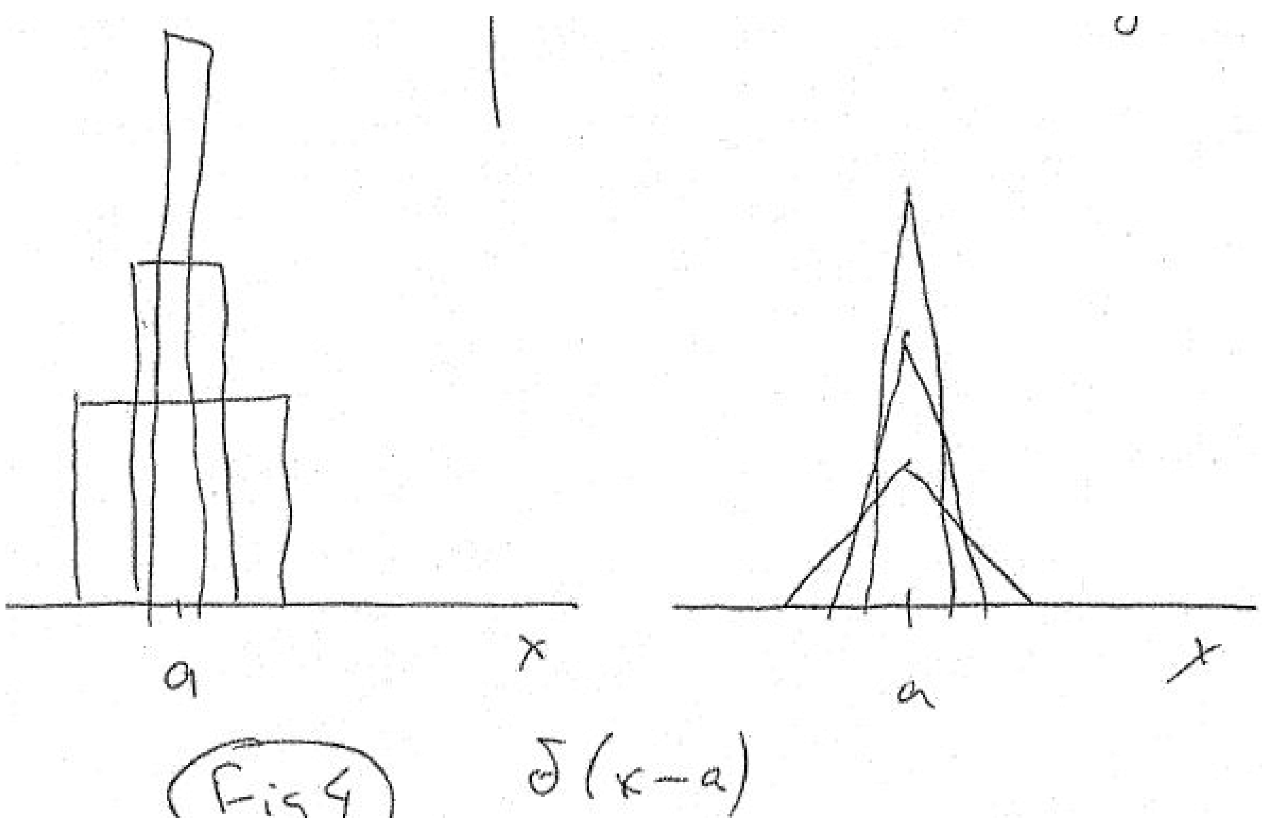

Figure 3.6: Two examples of a peak that can become a delta-function in the right limit

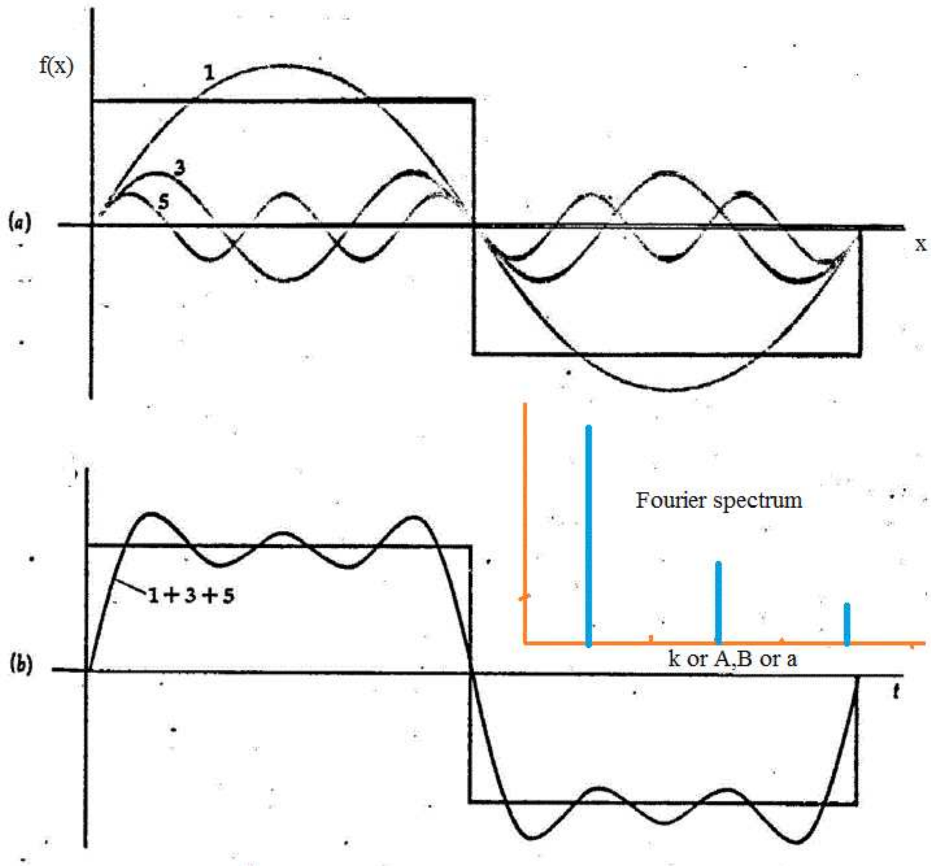

Figure 3.7: a) and b): Periodic square function $f(x)$ and its reconstruction from the first three harmonics. It is easy to see how the agreement is improved if more harmonics are included. Inset: the spectrum, i.e. the squares of absolute values of the Fourier transform $f(k)$ or of the Fourier coefficients A_n, B_n or a_n.

Chapter 4

Quantum Wave Mechanics

First, a few notes on Chapter 2:

a) Visualize $\lim_{L\to\infty}\int_{-L}^{+L} e^{ikx}dk$ vs. superposition of many sine waves that all have one thing in common

b) FT/FS enable us to synthesize a wave of arbitrary shape out of right amounts and phases of sines and cosines. How can we determine those "right amounts and phases"?

recall:

$$F(k) = (1/\sqrt{2\pi})\int f(x)e^{-ikx}dx$$

Then it is easy, using our (newly acquired, maybe) knowledge of the δ-function, to see that

$$(1/\sqrt{2\pi})\int F(k)e^{ikx}dk = f(x)$$

When the "spectrum" $F(k)$ happens to be a sum of discrete, equidistant peaks:

$$F(k) = \sum_{-\infty}^{\infty}\sqrt{2\pi}a_n\delta(k-nk_1)$$

it is easy to see that the resulting $f(x)$ will be periodic with period $2L = 2\pi/k_1$, described by a Fourier series:

$$f(x) = \sum_{n=0}^{\infty}A_n\cos\frac{n\pi x}{L} + \sum_{n=1}^{\infty}B_n\sin\frac{n\pi x}{L} = \sum_{-\infty}^{+\infty}a_n e^{in\pi x/L}$$

The 'base' functions $e^{in\pi x}$ satisfy an obvious (and very useful) **orthonormality** condition:

$$\frac{1}{2L}\int_{-L}^{+L} e^{in\pi x/L}e^{-im\pi x/L} = \delta_{mn}$$

This enables a determination of the coefficients: multiplying the expansion of $f(x)$ by $e^{-im\pi x/L}$, and integrating over x, one gets

$$a_m = \frac{1}{2L}\int_{-L}^{+L} f(x)e^{-im\pi x/L}$$

also: spectrum not invertible"

c) contemplate the similarity of Dirac delta and Kronecker delta

$$\int f(x)\delta(x-y)dx = f(y)$$

$$\sum_n f_n\delta_{nk} = f_k$$

4.1 Free particle with definite momentum:

traveling waves: to satisfy both the Planck/Einstein condition $E = hf$ and the deBroglie relation $\lambda = h/p$, we construct a plane wave:

$$\psi(x,t) = Ae^{i(kx-\omega t)} = Ae^{i(px-Et)/\hbar} = Ae^{i(x/\lambda - t/T)2\pi}$$

with $p = \hbar k$, $k = 2\pi/\lambda$, and $E = E(p)$ ($\omega = \omega(k)$). $\hbar = h/2\pi$ (or Physics department coffee bar [unfortunately canceled].)

Food for thought:

a) from the three forms of $\psi(x,t)$ select the one best suited for the consideration of the periodicity (recall that function $f(t)$ is periodic with period T if for any value of t

$$f(t+T) = f(t)$$

then the one that is simplest, and then the one that is closest to physics interpretation

b) Connect the three forms above with the concepts of wave function, period, wavelength, wave number, angular frequency, energy, momentum, Planck constant, Boltzman constant, and with the names Planck, Einstein and deBroglie.

c) Complex numbers appreciation here, and elsewhere (see Review of Math).

4.1.1 Wave Packets to describe a Localized Particle:

physics: localization in the x-space vs. localization in the p-space (k-space)

math: the probability amplitude F(k) and the probability amplitude f(x) are related by the Fourier transform:

$$f(x) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty} F(k)e^{ikx}dk \qquad F(k) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty} f(x)e^{-ikx}dx$$

where F(k) is the "cooking recipe" specifying the amount (and phase) of the momentum $\hbar k$ in the wave packet.

4.1.2 Relation of uncertainty I:

from counting number of wiggles in a finite region, and estimating the uncertainty in the count to be at least 1/10 of a wiggle, we get

$$\delta_x \delta_p \geq h/10$$

(see Figure 4.4) (doing the same in the (t,f) domain, we obtain the 'acoustical Heisenberg':

$$\delta_t \delta_f \geq 1/10$$

4.1.3 Relations of Uncertainty II:

math: for any two variables x, k related by a Fourier transform it is possible to show [1] that

$$\delta_x \delta_k \geq 1/2$$

. notes:

It follows that

$$\delta_x \delta_p \geq \hbar/2$$

This is not far off from the Uncertainty I !

It also follows that

$$\delta_E \delta_t \geq \hbar/2$$

but interpretation needs some care. Also, there is an interesting connection to line widths and lifetimes. And in acoustics, we get

$$\delta_t \delta_f \geq 1/4\pi$$

As we shall see, interpretation of **all** uncertainty relations needs a lot of care.

Sometimes $\delta q = \infty$. Even in this case, a restriction on the uncertainty of k can be found [2].

Deep down, the uncertainty relations result from non-commuting operators: more about this (and also about the original Heisenberg argument about disturbing the system!) in the section on Uncertainty Relations III.

All this is just a tip of the iceberg (vacuum fluctuations and polarization of vacuum and more).

4.1.4 Examples

Example 1: a flat rectangular packet

$$f(x) = \sqrt{\frac{1}{L}} \quad \text{in} \quad (-\frac{L}{2}, \frac{L}{2}) \quad \Rightarrow \quad F(k) = \sqrt{\frac{2}{\pi L}} \frac{\sin(kL/2)}{k}$$

[1] see E.H.Kennard,Z.Phys.44 (1927) 326

[2] H.J.Landau and H.O.Pollak, Bell Syst. Tech.J. 40 (1961) 65

The packet is centered in momentum space on k=0. Therefore, it does not move —it just diffuses. The packet peaks at $k = 0$, but it has many "lobes" all the way to $\pm\infty$. This is the consequence of the sharp edges of the packet in x-space. It is amusing to see the 0/0 behaviour at $k = 0$. It is also amusing to check the uncertainty relation.
Note: obviously, a flat rectangular packet in k-space will produce a similar peak with lobes in the x-space. However, the time dependence will be different in the two cases.

Example 2: a chopped beam

$$f(x) = \sqrt{\frac{1}{L}} e^{ik_0x} \text{ in } (-\frac{L}{2}, \frac{L}{2}) \quad \Rightarrow \quad F(k) = \sqrt{\frac{2}{\pi L}} \frac{\sin((k-k_0)L/2)}{(k-k_0)}$$

Same as Example 1, but the packet is now moving with momentum $\hbar k_0$.

Example 3: the Gaussian wave packet [3]

$$F(k) = \sqrt{\frac{2a}{\sqrt{2\pi}}} e^{-a^2(k-k_0)^2} \quad \Rightarrow \quad f(x) = \frac{1}{\sqrt{a\sqrt{2\pi}}} e^{ik_o x} e^{-x^2/4a^2}$$

Interpretation: $p = \hbar k_0$, $\sigma_x = a$, $\sigma_k = 1/2a \;\Rightarrow\; \sigma_x \sigma_p = 1/2$, i.e. $\sigma_x\sigma_p = \hbar/2$. The product of the two uncertainties is the minimum consistent with the Relation of Uncertainty.

It is very useful to visualize the wave packet as a little "screw" with x along $\mathrm{Re}f(x)$, y along $\mathrm{Im}f(x)$ and the particle moving along z. Thanks to the complex numbers, $f(x)$ is wavy as required by deBroglie, but does not ever go through zero (as required by the probability interpretation of a free particle. Note also the the width of the wave packet has nothing to do with the size of the particle!

4.1.5 Time development of the wave packet for a free particle

The relations that explain the deep connections between wavelength, period, momentum, energy, wave number and angular frequency are so important that we repeat them here::

$$f(x,t) = Ae^{2\pi i(x/\lambda - t/T)} = Ae^{i(kx-\omega t)} = Ae^{2\pi i(px-Et)}$$

4.1.6 The phase velocity and group velocity

For a plane wave: $f(x,t) = e^{i(kx-\omega t)} = e^{ik(x-v_{phase}t)}$, where $v_{phase} = \omega/k$.
At any time t, the wave packet

$$f(x,t) = \frac{1}{\sqrt{2\pi}} \int F(k) e^{i(kx-\omega(k)t)} dk \quad \text{(note that for free particle } F(k,t) = F(k))$$

[3]recall: a Gaussian distribution with mean y_0 and standard deviation σ is

$$\frac{1}{\sigma\sqrt{2\pi}} e^{-(y-y_0)^2/2\sigma^2}$$

The meaning of σ is: "the half-width at 61% of maximum".

will have the maximum at a point where

$$\frac{d(kx - \omega(k)t)}{dk} = 0 \quad \Rightarrow \quad x = \frac{d\omega}{dk} t \quad \Rightarrow \quad v_{group} = \frac{d\omega}{dk}$$

The concepts of phase and group velocity are illustrated in Figure 4.1

3) **Important example of Gaussian wave packet**
for a Gaussian packet and $\omega(k) = \omega_0 + v(k - k_0) + \beta(k - k_0)^2$
(these are the first three terms of a Taylor expansion, i.e.

$$v = d\omega/dk|_0 \quad \beta = 1/2 \ d^2\omega/dk^2|_0$$

A little (in fact, a moderate amount of) algebra results into:

$$f(x,t) = e^{i(k_0 x - \omega_0 t)} \sqrt{\frac{\pi}{a^2 + i\beta t}} e^{-(x-vt)^2/4(a^2+i\beta t)}$$

and the corresponding magnitude is in Peleg eq. 3.15.7 . This is given here as an example how complex it sometimes is to describe such a simple object as a free particle. What is important is to be able to interpret the math:

This is a particle moving with momentum $p_0 = \hbar k_0$, corresponding to a Gaussian with mean $= x - vt$ and standard deviation

$$\sigma = a\sqrt{1 + t^2/\tau^2} \quad \text{where} \quad \tau = a^2/\beta$$

notes:

for a relativistic particle ($E = pc$), you get $v = c$ and no spreading ($\beta = 0$). Note that our β is not the usual $\beta = v/c$.

for a non-relativistic particle ($e = p^2/2m$), you get $v = p/m$ and $\tau = 2ma^2/\hbar$. This can be very brief for microscopic particles, but extremely long for even very small microscopic objects. Notice that it is proportional to the square of the original position uncertainty.

The expression for σ can be written as

$$\sigma = \sqrt{\sigma_0^2 + \sigma_1^2}$$

where $\sigma_0 = a$ is the original uncertainty in position at time $t = 0$, and $\sigma_1 = \beta t/a = t\sigma_p/m = \sigma_v t$ is the uncertainty due to the uncertainty in the momentum. Note that $\sigma = \sigma_0$ initially, and $\sigma = \sigma_1$ much later - just like at the Boston marathon!

4.1.7 Particle in a Box revisited

This is a very simple but very useful "playground" of Quantum Mechanics (see Fig. 8). Standing waves with

$$L = n\lambda_n/2$$

immediately yield quantization of energy

$$E_n = n^2 E_1$$

where $E_1 = h^2/8mL^2 \neq 0$, in agreement with the relations of uncertainty

HW: Use the Uncertainty Relation to estimate the energy of the ground state of the Simple Harmonic Oscillator. (hint: use the Uncertainty Relation to express $< p^2 >$ in terms of $< x^2 >$, and then look for a minimum of E).

4.1.8 Elementary Quantum Mechanics and Relativity:

(optional but very interesting)

a) **calculation of Doppler shift using a radiative decay:**

This example and associated homework provide a wealth of quantum physics, relativity and numerical methods for fun and profit. Consider a decay of a particle with (mass,momentum,energy)=$(m_1, \vec{p}_1$ into a particle with $(m_2, \vec{p}_2, E_2)$ and a photon with $(0, \vec{p}, E)$. Recall the Lorentz factors

$$\beta_1 = \frac{v_1}{c} = \frac{p_1 c}{E_1}$$

$$\gamma_1 = \frac{1}{\sqrt{1-\beta_1^2}} = \frac{E_1}{m_1 c^2}$$

Now, the energy and momentum conservation give

$$E_1 - E = E_2$$

$$c(\vec{p}_1 - \vec{p}) = c\vec{p}_2$$

When you subtract the square of the second equation from the square of the first one, you should get (after recalling that $|\vec{a} + \vec{b}|^2 = a^2 + b^2 + 2ab\cos\theta$)

$$E = \frac{m_1^2 c^4 - m_2^2 c^4}{2m_1 c^2} \frac{1}{\gamma_1(1 - \beta_1 \cos\theta)}$$

Physical interpretation of this result becomes clear if we re-write it as

$$E = E_0 \frac{\sqrt{1-\beta_1^2}}{1 - \beta_1 \cos\theta}$$

where E_0 is the energy of the photon when the parent particle is at rest, i.e. it is the energy of the photon as seen from the rest-frame of the parent particle.

And now comes the gem: the relation between the photon frequency f as seen from the laboratory frame, and the frequency f_0 as seen from the rest frame of the parent particle is obtained by using

$$E = hf, E_0 = hf_0$$

which yields the Doppler formula

$$f = f_0 \frac{\sqrt{1-\beta_1^2}}{1-\beta_1 \cos\theta}$$

HW: fill in the missing steps.

b) **calculation of the gravitational redshift:**
This is a much simpler but equally remarkable connection of elementary quantum physics to relativity (this time, General Relativity). Consider light of frequency f_0 emitted downwards from a tower of height x. At the bottom, each photon will have energy $E = E_0 + gxE_0/c^2$. This immediately yields the gravitational redshift

$$(f - f_0)/f_0 = gx/c^2$$

Note that this does not depend on h. On Earth, with $x = 20m$, $gx/c^2 = 2.10^{-15}$. This has been measured(!) using the Mössbauer effect.

4.2 Figures

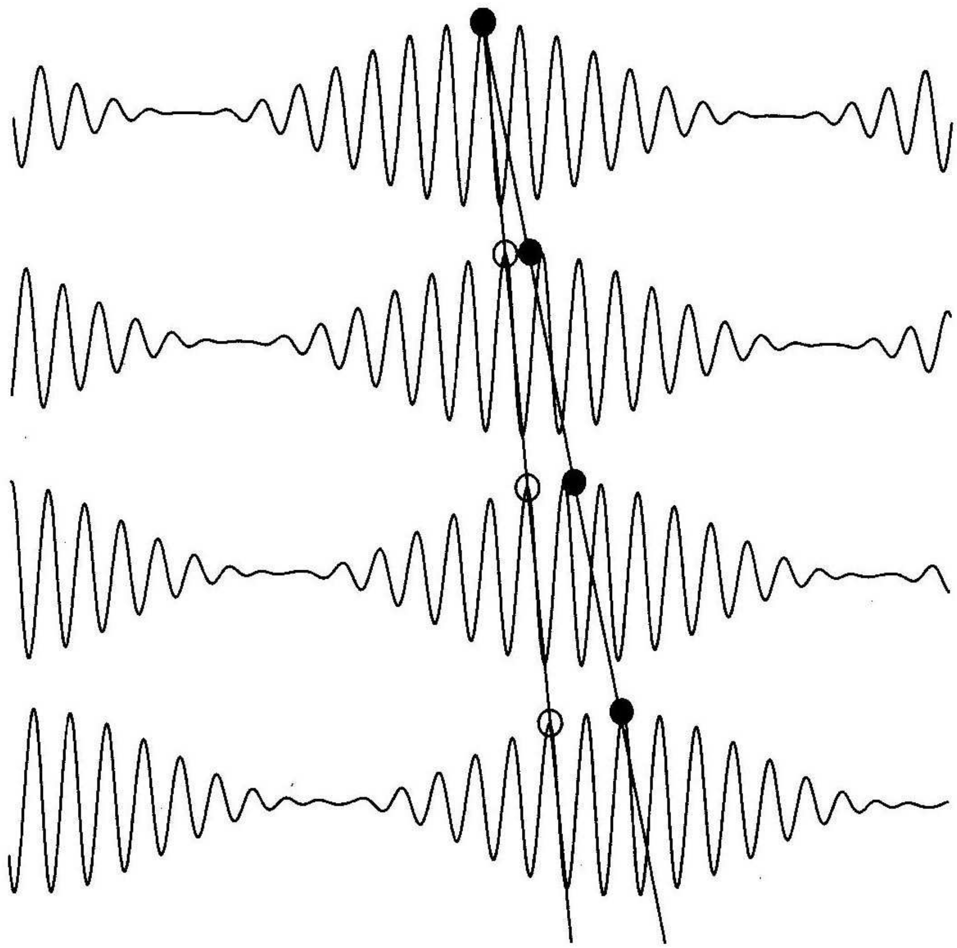

FIGURE 6.6 Discrete wave packet animation with time increasing from top to bottom. Open circles identify a point of constant phase, which moves at the phase velocity. Filled circles identify the peak of the envelope, which moves at the group velocity.

Figure 4.1: Illustration of the phase velocity and group velocity

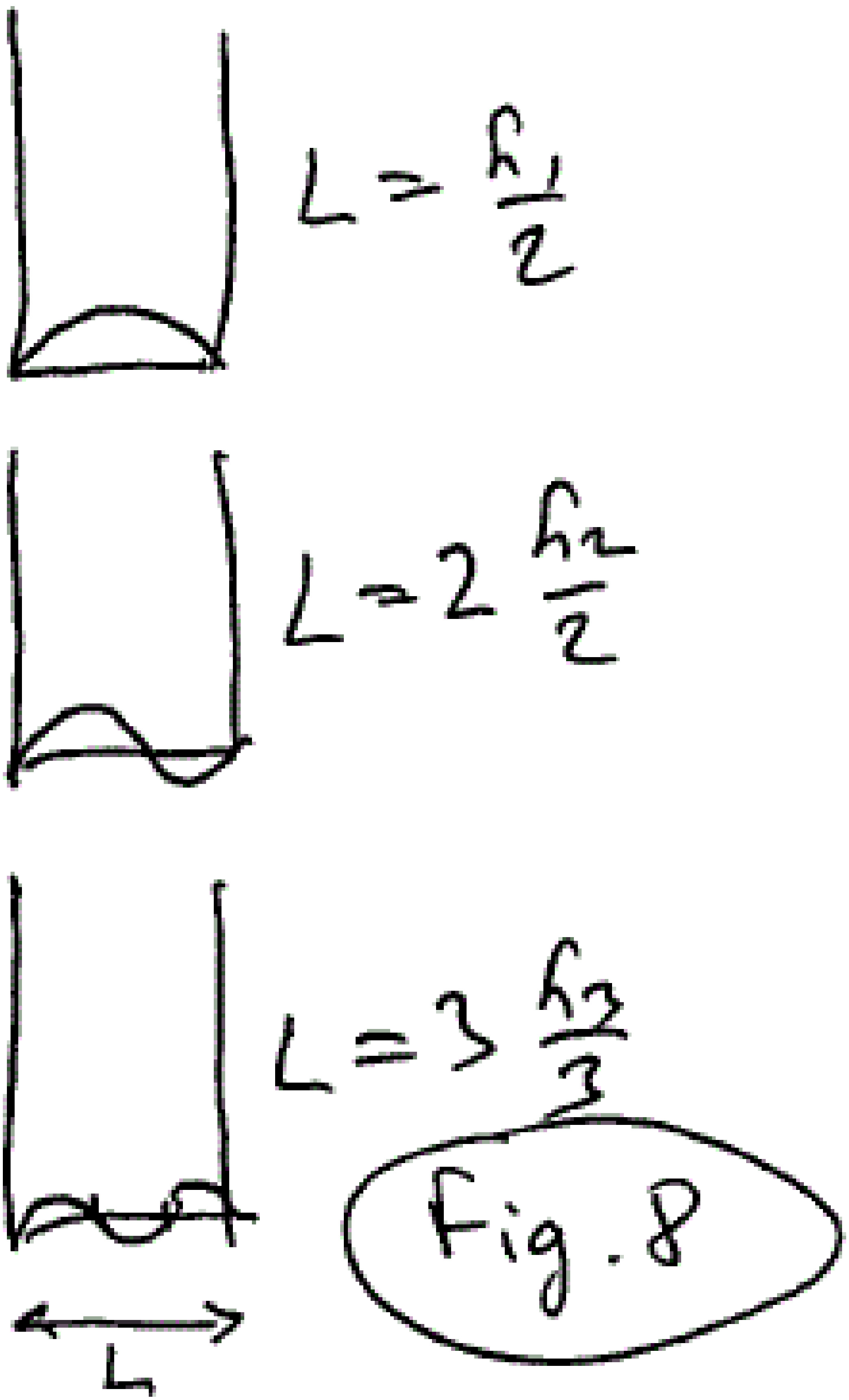

Figure 4.2: This simplest of all diagrams has an awful typo. I am leaving it here as a contribution to the psychology of typos; a better potential box is on Figure **??**infVsFiniteWell

Figure 4.3: A better potential box than Figure 4.2. The finite well on the right is discussed in Chapter 5.

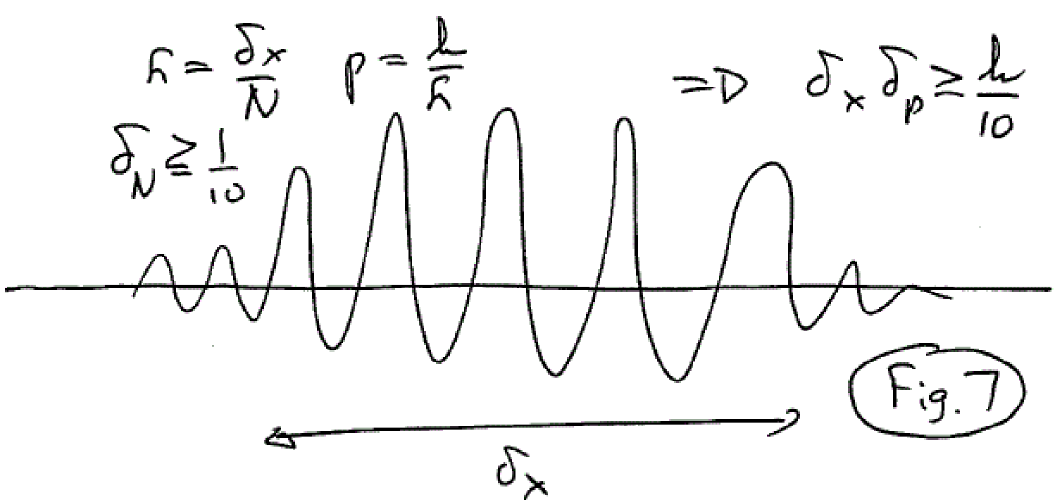

Figure 4.4: Illustratiom of a “poor man’s Heisenberg. Handwaving but basically correct and numerically close to the real thing.

Chapter 5

Quantum Mechanics I

To progress towards a more detailed quantum mechanics, we have two questions to deal with:
a) what are the properties of the state described by a particular function $\psi(x)$
b) what is the "equation of motion" for $\psi(x,t)$

5.1 More properties of the wave function

In quantum physics, the wave function $\psi(x,t)$ describes the system completely. This means we can use it to determine not just the probability density $P(x,t) = |\psi(x,t)|^2$ but also the possible values a_i of any physical observable A and their probabilities. This is done by a fairly involved and completely new procedure in three steps:

5.1.1 Observables ad Operators

to every observable A we assign an operator $\hat{A}$ that operates on a wave function and produces another function:

$$\hat{A}\psi(x,t) = \phi(x,t)$$

Examples: for position we have (don't laugh) $\hat{x} = x$, the operator of momentum is $\hat{p} = -i\hbar\partial/\partial x$

For now, you should take this as "experimental" facts; we will see the deep logic motivating these choices later in this course.

5.1.2 The Eigenequation

The only possible values that observable A can have are solutions of the equation

$$\hat{A}\psi_a(x,t) = a\psi_a(x,t)$$

This equation is called an eigen-equation, and its solutions are the eigenvalue (a) and corresponding eigenfunction (ψ_a).

Example 1: for the function $\psi_1(x) = \sin(px/\hbar)$ we have

$$\hat{p}\psi_1(x) = -i\hbar \frac{d\ \sin(px)/\hbar)}{dx} = -ip\ \cos(px/\hbar)$$

Therefore, ψ_1 is not an eigenfunction of momentum. Similarly for $\psi_2(x) = \cos(px/\hbar)$

Example 2: for the function $\psi_3(x) = e^{+ipx/\hbar}$ we get

$$\hat{p}\psi_3 = p\psi_3$$

and ψ_3 is an eigenfunction of momentum, with eigenvalue p

similarly, for the function $\psi_4(x) = e^{-ipx/\hbar}$ we get

$$\hat{p}\psi_4 = -p\psi_4$$

and ψ_4 is an eigenfunction of momentum, with eigenvalue $-p$

Example 3: HW: check that all four functions $\psi_1(x)$ - $\psi_4(x)$ are eigenfunctions of kinetic energy, all with the same eigenvalue $E = p^2/2m$. This is our first encounter with the important concept of "degeneracy", where more than one eigenfunction correspond to the same eigenvalue.

Example 4: As HW, contemplate the eigen-equation for the position operator $\hat{x}$ and its solution. Note that this is very simple, but also very subtle (and very important)!

$$\hat{x}\psi_0(x) = x\psi_0(x) = x_0\psi(x)$$

the solution: wave function that is an eigen-function of operator $\hat{x}$ with eigenvalue x_0 is

$$\psi_0(x) = \delta(x - x_0)$$

5.1.3 Fundamental expression for the QM Probability

If the system is in the state described by ψ and we measure the observable A, the probability amplitude for obtaining the particular value (a) is

$$\int_{-\infty}^{\infty} \psi_a^*(x)\psi(x)dx$$

Immediately after finding the value "a", the state of the system will change from ψ to ψ_a. This is the (in)famous "collapse" of the wave function. Much more on this (and on the whole "measurement problem") later in this course.

5.2 The wave equation

The equation describing the time development of the wave function between measurements is the celebrated Schroedinger equation [1]:

[1]Remarkably, Schrodinger's interpretation of his own equation was wrong, and reaction by his competitor Heisenberg and others was not enthusiastic, to say the least. But he had the last laugh ...

$$i\hbar\frac{\partial\psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\psi(x,t)}{\partial x^2} + V(x,t)\psi(x,t)$$

This may look very complicated, but once you recall that the operator of momentum is $\hat{p} = -i\hbar\partial/\partial x$ you can see right away that the right hand side is simply

$$(\frac{\hat{p}^2}{2m} + \hat{V})\psi = \hat{E}\psi = \hat{H}\psi$$

On the other hand we shall see that there is a close connection between $i\hbar\frac{\partial}{\partial t}$ and energy.

In words, the Schrodinger equation says: the rate of change of the wave function with time is given by the operator of kinetic plus potential energy, i.e. operator of the total energy $\hat{E}$, also known as the Hamiltonian $\hat{H}$, operating on the wave function.

Note that in contrast to Newton's law, the Schrodinger equation is first-order in time, so that $\psi(x,t_0)$ suffices to specify $\psi(x,t)$.

Simple as it may be, the equation is so difficult to solve that an analytic solution is known only for a handful of cases; the rest of the problems must be solved using all kinds of approximations, or by a brute force (numerically).

5.2.1 Separation of variables

A very important method, both theoretically as well as in practice, of reducing the complexity of the problem is available for time-independent potentials: $V(x,t) = V(x)$. By using a beautiful trick we will encounter several times (also in EM) one can easily show that there are particular solutions of the Schroedinger equation that have the form

$$\Psi(x,t) = \psi(x)\phi(t)$$

where ψ and ϕ are solutions of the ordinary differential equations

$$\frac{d\phi(t)}{dt} = -i\frac{E}{\hbar}t\ \phi(t)$$

and

$$\hat{E}\psi(x) = E\psi(x)$$

where E is an arbitrary (for now) constant
The first equation has a ready solution, the same for any problem, namely:

$$\phi(t) = e^{-iEt/\hbar}$$

The second equation is the difficult one, and it must be solved for the particular potential $V(x)$ that appears in the Hamiltonian. Note that it really is an eigen-equation for energy, also called Time-Independent Schroedinger Equation, or TISE, as opposed to TDSE. So the "arbitrary" constant is really the energy E, and the equation should be written in the form

$$\hat{H}\psi_E(x) = \hat{E}\psi_E(x) = (\frac{\hat{p}^2}{2m} + \hat{V})\psi_E = E\psi_E(x)$$

where $\psi_E(x)$ is the energy eigenfunction corresponding to energy E.

The highlight of all this is that since the equation is linear, a general solution can then be assembled of the particular solutions:

$$\Psi(x,t) = (\int dE \ or \ \sum_E) \quad g(E)\ \psi_E(x)\ e^{-iEt/\hbar}$$

with the "weighting function" $g(E)$ chosen to reproduce the initial conditions of the given problem. Note that another name for $g(E)$ is therefore the "probability amplitude" for energy, $|g(E)|^2$ is the probability density, and $|g(E_n)|^2$ would be the probability of energy E_n.

5.2.2 General properties of the solution

Before we discuss specific solutions of specific problems, it will be useful to pause for a moment to think about their general properties. Recast the TISE as

$$\frac{d^2\psi(x)}{dx^2} \sim -(E-V)\psi(x)$$

When particle moves in the classically-allowed region, i.e. $E > V$, the equation implies that the second derivative of ψ has opposite sign to that of ψ itself. A minute with a pen and pencil will show you that the behavior will be oscillatory, in agreement with Dr.(also Prince) deBroglie. The wavelength of the oscillations will vary with the value of (E-V) but as long as it is positive, ψ will oscillate.

On the other hand, the region with $E < V$ is classically forbidden - the kinetic energy is negative, so momentum is imaginary! But the Schrodinger equation does have a non-trivial solution, with second derivative of the same sign as ψ. And again, you should be able to convince yourself that in this case it implies an exponentially-suppressed penetration of the particle into the forbidden region, possibly from both sides. And this is a far-reaching conclusion, obtained quite early in our discussions!

5.2.3 Consequences for quantization

But there is more we can already deduce and learn. Imagine a particle in a potential well as illustrated on Figure 4.3, together with the qualitative behavior of its wave function we now understand. We will easily prove (next section) that at the points where particle crosses between allowed and forbidden regions, the wave function and its first derivative must be continuous (as long as the potential there is finite). It turns out that this is only possible at selected values of the energy: $E_1, E_2, E_3, ...$ This is the physical origin of quantization of the atomic levels, stability of the atom, and much more!

On the other hand, if the particle is not restricted from both sides, the conditions are achievable for any energy, and particle is "unbound" - free to move, but not "really" free if $V(x) \neq \ const.$

5.2.4 Current of probability density

Multiply the Schrodinger equation by ψ^* and subtract the complex-conjugate of this construct. Show (as HW) that this yields

$$\frac{\partial \rho(x,t)}{\partial t} = -\frac{\partial j(x,t)}{\partial x}$$

where $\rho(x,t) = \psi\psi^*$ is the familiar probability density, and

$$j(x,t) = (\hbar/m)\ Im[\psi^*(x,t)\frac{\partial \psi(x,t)}{\partial x}$$

Integrating the equation over x from a to b gives

$$dP_{ab}(t) = j(a,t) - j(b,t)$$

which shows that the interpretation of the function $j(x,t)$ is the "current (flux) of probability density". The differential and the integrated equations are the differential and integral expression of the conservation of probability. In particular, for a particular choice (which one?) of a and b, this implies conservation of normalization.

Recall the introduction of differential and integral conservation of electric charge in E&M.

HW: Using the polar form of the wave function: $\psi(x,t) = a(x,t)e^{i\phi(x,t)}$ show that:

a) the result for the current of the probability density of a free particle makes perfect sense.

b) to obtain non-zero current of probability density, the wave function must be "non-trivially complex".

5.2.5 (Dis)continuity of the wave-function

1) The wave function itself must be continuous everywhere (otherwise the current of probability density would have a singularity). We express this as

$$disc_a\psi(x) = \lim_{\epsilon\to 0}[\psi(a+\epsilon) - \psi(a-\epsilon)] = 0$$

2) The discontinuity of the first derivative is obtained from the Schrodinger equation:

$$\frac{\partial \psi}{\partial x}|_{a+\epsilon} - \frac{\partial \psi}{\partial x}|_{a-\epsilon} = \int_{a-\epsilon}^{a+\epsilon} dx \frac{\partial^2 \psi}{\partial x^2} = \frac{2m}{\hbar^2}\int_{a-\epsilon}^{a+\epsilon} dx[V(x) - E]\psi(x)$$

Therefore the derivative is continuous at $x = a$ for a finite potential $V(a)$, and for a singular potential $V(x) = \lambda\delta(x-a)$ we get

$$disc_a\frac{\partial \psi}{\partial x} = \frac{2m\lambda}{\hbar^2}\psi(a)$$

(the parameter λ represents the "strength of the singularity".)

5.2.6 Piece-wise constant potentials

a) The simplest case of this important category is when there is only one piece: $V(x) = V_0$. This means the particle is free, and we have already obtained the wave function - convince yourself that it indeed satisfy the Schroedinger equation (as well as the demands of Prof. Einstein on the period, and Prof. deBroglie on the wavelength). The wave packet we introduced as an example of the Fourier Transform, is now seen as a special case of the assembly of the general solution from the particular solutions obtained by the separation of variables.

b) The second simplest case: $V(x) = V_0$ on an interval, and $V(x) = \infty$ anywhere outside the interval is nothing but the "particle-in-the-box" we discussed earlier. It is educational to think how this is modified when the box is not infinitely deep.

c) The general piece-wise-constant potential is also the most useful: it contains reflection off a potential wall, scattering off a potential well, and - most importantly - tunneling through a potential barriere. In any of these cases, the solutions are analytically known in any region of the constant potential:
where $E > V$, the wave function is

$$\psi_E(x) \sim e^{\pm ikx} \quad where \quad k^2\hbar^2/2m = E - V$$

and for the forbidden region

$$\psi_E(x) \sim e^{\pm kx} \quad where \quad k^2\hbar^2/2m = V - E$$

Assembling the overall wave function from the individual segments with constant potential is easy because the solutions of each segment is trivial. Demanding the continuity of ψ and its derivative $d\psi/dx$ at the entry and exit of the barrier yields connects the segments into the final wave function that is far from trivial!.

And finally the sweet reward: all this is for the stationary case of one particular solution. Now assemble a real, moving wave packet, and sit back and watch what "really happens" (DEMO). The variety of effects is amazing, and covers much of modern quantum electronics!

Note also that many potentials can be approximated in a piece-wise constant manner. In principle, this can get you an easy approximate solution of the corresponding problem.

5.3 Filling in the details

5.3.1 Re 5.2.1: Separation of variables

Just do it: plug $\Psi(x,t) = \psi(x)\phi(t)$ into the Schrodinger equation, and you get

$$i\hbar\psi(x)\frac{d\phi(t)}{dt} = -\frac{\hbar^2}{2m}\phi(t)\frac{d^2\psi(x)}{dx^2} + V(x)\psi(x)\phi(t)$$

when you divide this equation by

$$\Psi(x,t) = \psi(x)\phi(t)$$

you will get

$$i\hbar\frac{d\phi(t)}{dt}\frac{1}{\phi(t)} = -\frac{\hbar^2}{2m}\frac{1}{\psi(x)}\frac{d^2\psi}{dx^2} + V(x)$$

A little reflection shows that this equation can only be true if both sides are separately equal to the same constant because the first term is only function of t and second term depends only on x. Obviously that constant should be called E ...

5.3.2 Re 5.2.4: Flux of probability density

Following the suggestion in the Text we get

$$i\hbar\Psi^*(x,t)\frac{\partial\Psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m}\Psi^*(x,t)\frac{\partial^2}{\partial x^2}\Psi(x,t) + V(x)\Psi(x,t)\Psi^*(x,t)$$

$$-i\hbar\Psi(x,t)\frac{\partial\Psi^*(x,t)}{\partial t} = -\frac{\hbar^2}{2m}\Psi(x,t)\frac{\partial^2}{\partial x^2}\Psi^*(x,t) + V(x)\Psi^*(x,t)\Psi(x,t)$$

Now using $\rho(x,t) = \Psi\Psi^*$ for the probability density,

expressing $\frac{\partial^2\Psi(x,t)}{\partial x^2}\Psi^*(x,t)$ using the rule for a derivative of the product

$$\frac{\partial}{\partial x}[\Psi^*\frac{\partial\psi}{\partial x}]$$

and realizing that we assume the potential to be real (not complex),

you get the result in the text (I am leaving the nitty-gritty details for you as a delightful calculus exercise ...). As we shall see in the next paragraph, this is the differential form of conservation of probability.

Integrating the differential form

$$\frac{\partial\rho(x,t)}{\partial t} = \frac{\partial j(x,t)}{\partial x}$$

over the x interval (a,b) we get the integral form

$$dP_{a,b}(t) = j(a,t) - j(b,t)$$

5.3.3 Wave function in the Polar form

$$\Psi(x,t) = Re\Psi(x,t) + i\ Im\Psi(x,t) = a(x,t)e^{i\phi(t)}$$

Plugging the polar form into the expression for the flux of probability we get

$$j(x,t) = \frac{\hbar}{m}|a|^2\ Im\frac{\partial\phi(x,t)}{\partial x}$$

This explains the meaning of the concept of “non-trivially complex”.

Applying this on a free particle for which $\phi = px/\hbar$ yields the highly satisfying result $j = |a|^2 v$ i.e. the flux of probability is the probability density times velocity.

5.4 Applications

5.4.1 Potential step

a) forbidden region: not so forbidden when you take Dr. Schrodinger seriously (as you should)

b) quantum reflection off a cliff
The puzzle noted in the Figure Caption is addressed in the following very important Homework:

It can be shown (see Landau/Lifschitz' famous text on Quantum Mechanics) that for the potential

$$V(x) = \frac{V_0}{1 + e^{-\alpha x}}$$

the reflection coefficient is

$$R = (\frac{\sinh(\pi(k_1 - k_2)/\alpha)}{\sinh(\pi(k_1 + k_2)/\alpha)})^2$$

where $k_1(k_2)$ are the wave numbers at $x = +\infty(-\infty$. Recall that $\sinh(x) = (e^x - e^{-x})/2$.

5.4.2 Potential barrier

a) decaying wavefunction resuscitated (like a Phoenix from ashes)

If you are really motivated, find the transmission coefficient and show that for $k_2 = \sqrt{2m(V_0 - E)}$, barrier width a and $ka >> 1$, the transmission is $T \sim e^{-2k_2 a}$. This is the principle of the scanning electron microscope (see Figure).
b) non-classical scattering

5.4.3 Potential well

a) bound states

b) non-classical scattering

5.4.4 From atom to molecule and back

kindly assisted by the delta-function

This is the second very important Homework assignment of this section: study the behavior of this bound state for
a) small
b) large
value of λ. Calculations are not difficult, but you will learn a lot from even just a qualitative understanding (and you will come to appreciate/love the delta function :-) .

5.5 Figures

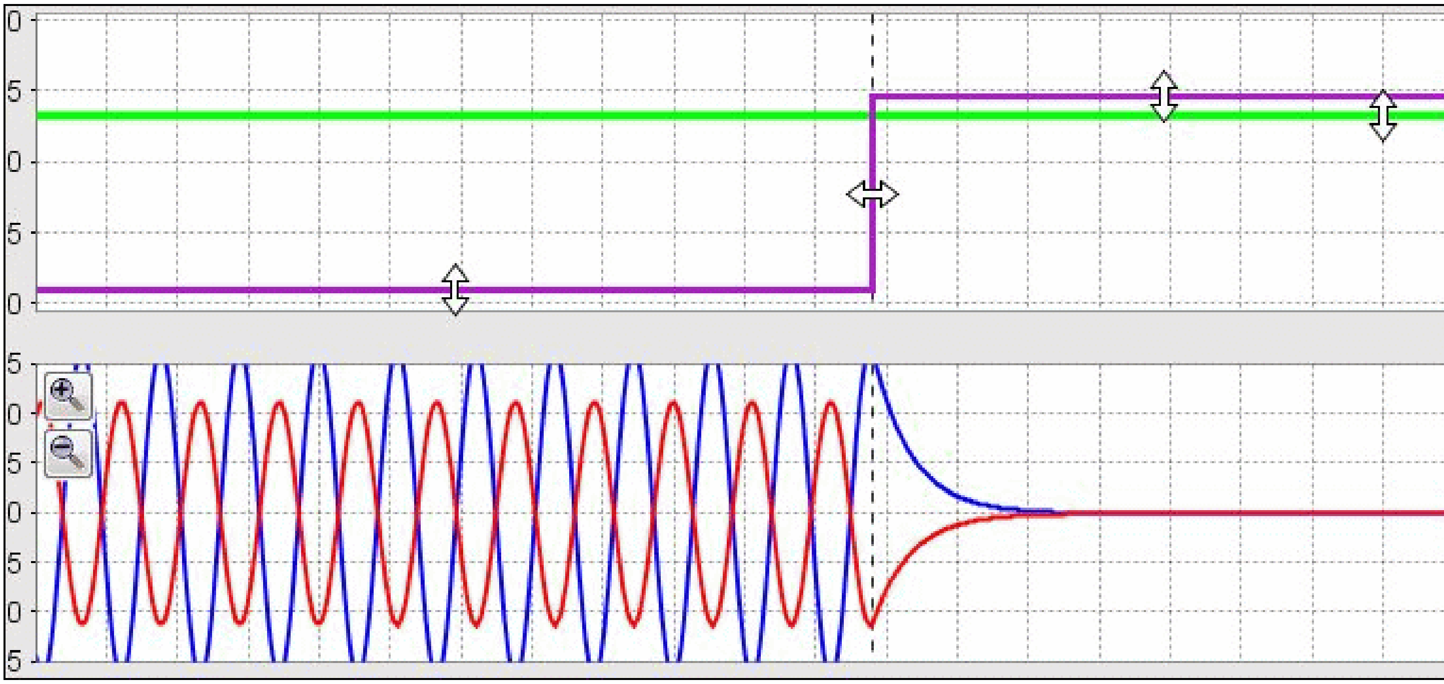

Figure 5.1: Top: red=potential V(x)=0 on the left (V(x)=V_0 on the right); green = particle energy $E < V_0$ so motion is classically forbidden
The wave function is $Ae^{ik_1 x} + Be^{-ik_1 x}$ on the left, $Ce^{-k_2 x}$ on the right
The continuity of $\psi(x)$ at $x = 0$ requires $A + B = C$
The continuity of $d\psi/dx$ at $x = 0$ requires $Aik_1 - Bik_1 = -Ck_2$
Since A is arbitrary, we have two equations for two unknowns, easily solved, giving the solution:
$\frac{B}{A} = \frac{k_1 - ik_2}{k_1 + ik_2} \quad \frac{C}{A} = \frac{2k_1}{k_1 + ik_2}$
and since $|B/A| = 1$ there is no transmission (of course: the "penetrating" wave is only trivially complex :)

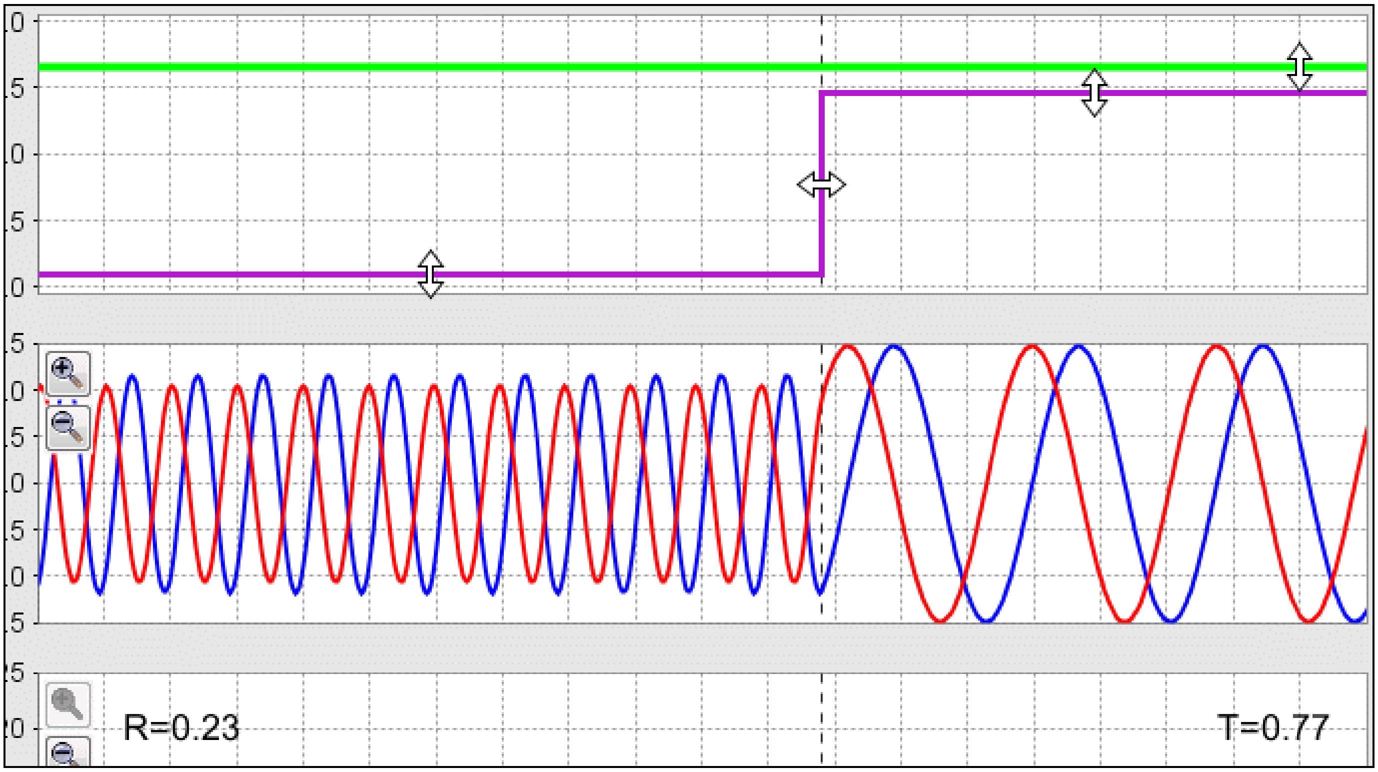

Figure 5.2: Particle hitting the "potential cliff" with EV_0 so the motion is classically allowed in the whole range of x. The wave function is $Ae^{ik_1x} + Be^{-ik_1x}$ on the left, Ce^{ik_2x} on the right. You can go through the above procedure step by step but the solution is immediately obtained by substituting ik_2 for $-k_2$ and the result is
reflection coefficient $R = \frac{k_1|B|^2}{k_1|A|^2} = \frac{(k_1-k_2)^2}{(k_1+k_2)^2}$
This seems all well and good until you realize that the same formula applies for particles coming from the right-hand side, i.e. going off the cliff.

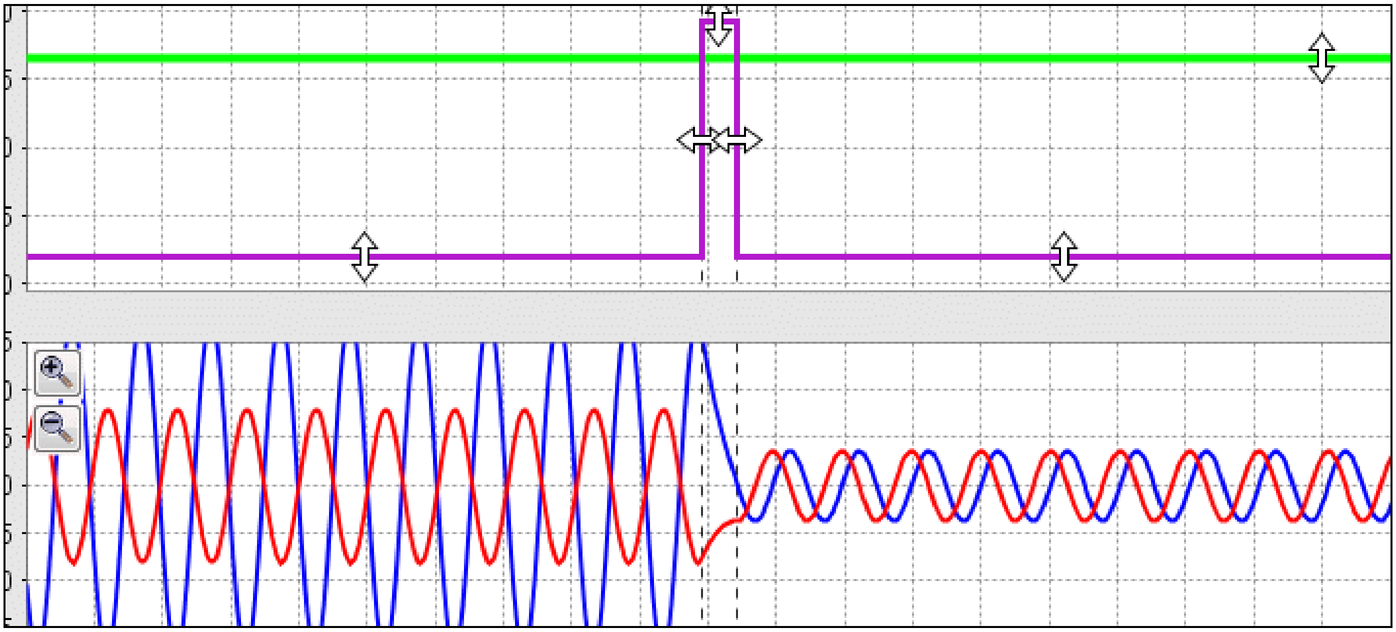

Figure 5.3: A stationary solution for barrier tunneling.

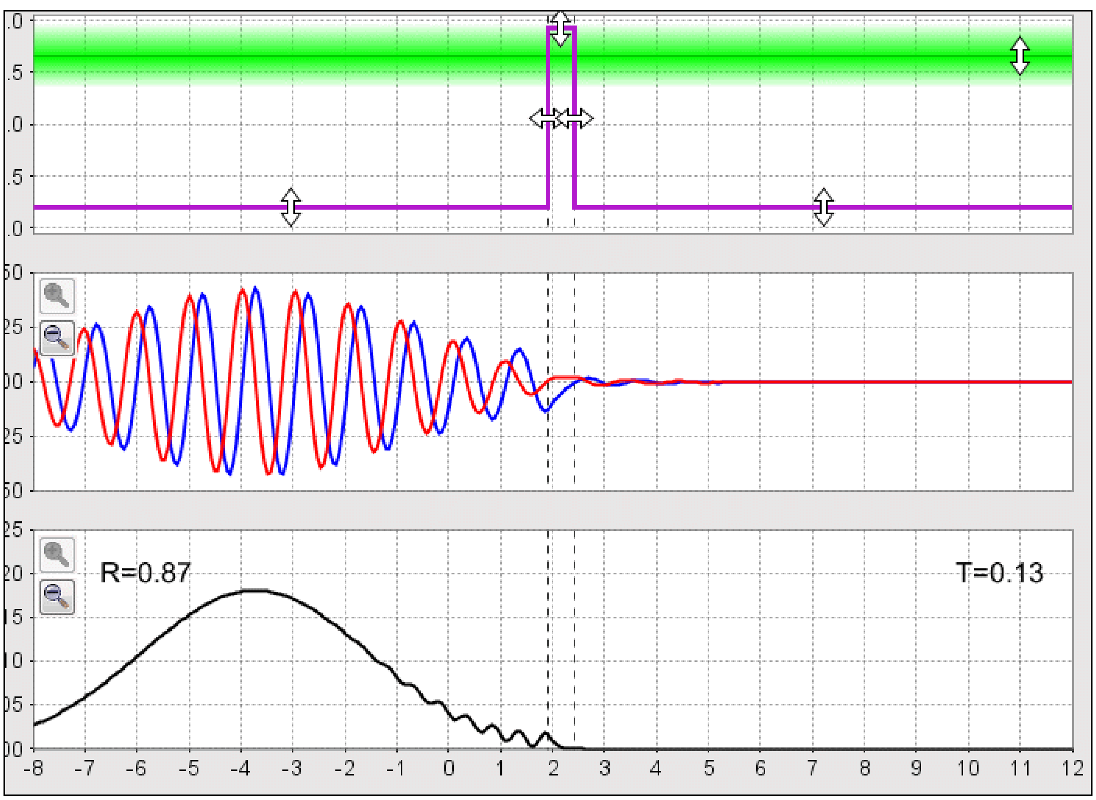

Figure 5.4: Wave packet traveling towards barrier

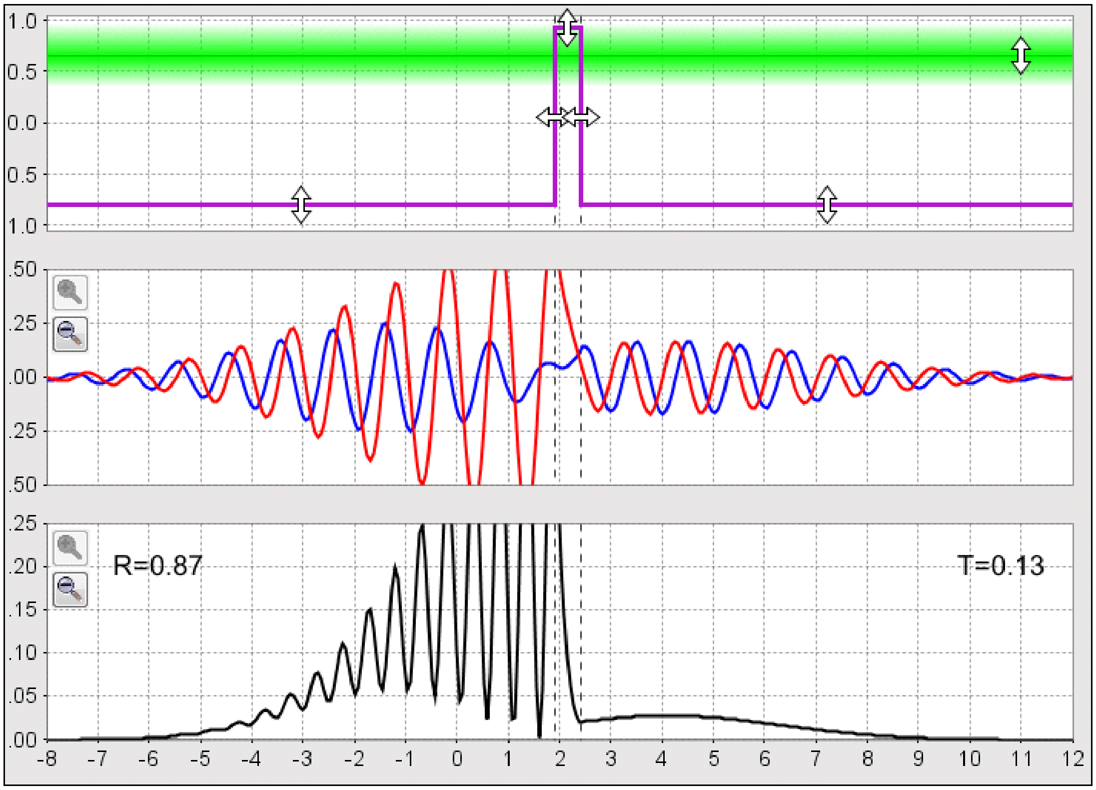

Figure 5.5: Wave packet tunnels through barrier

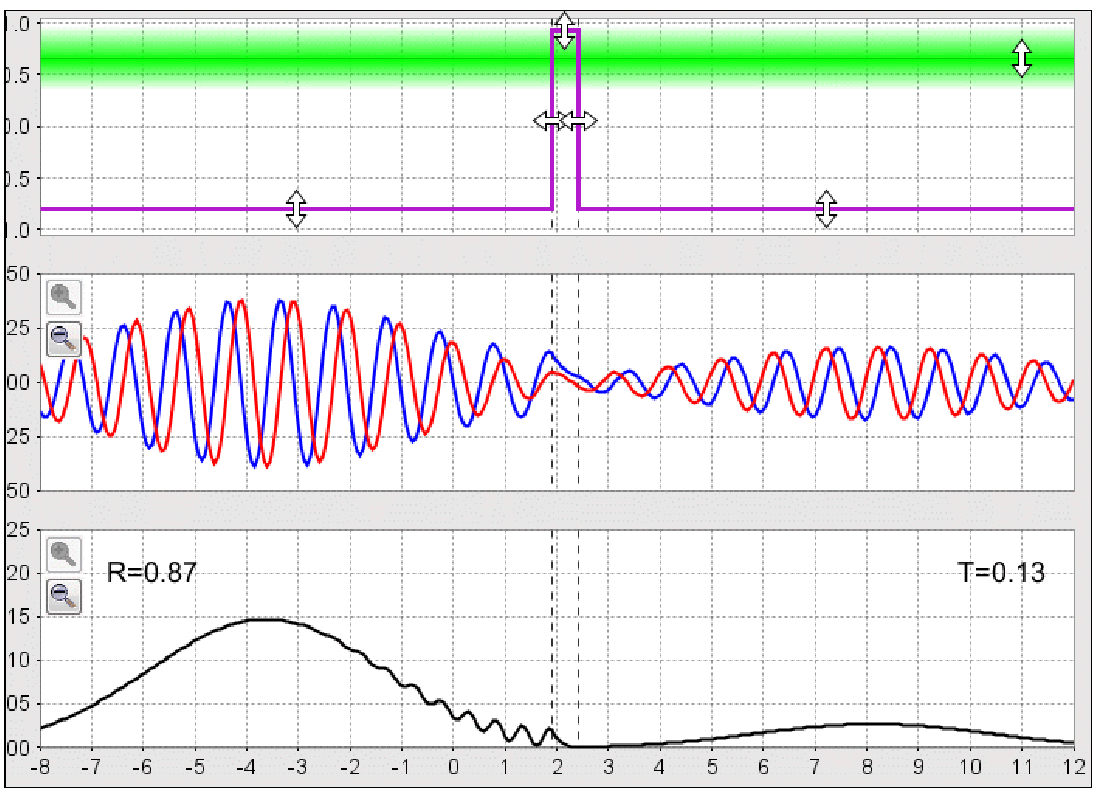

Figure 5.6: Wave packet reconstitutes itself into reflected and transmitted packets.

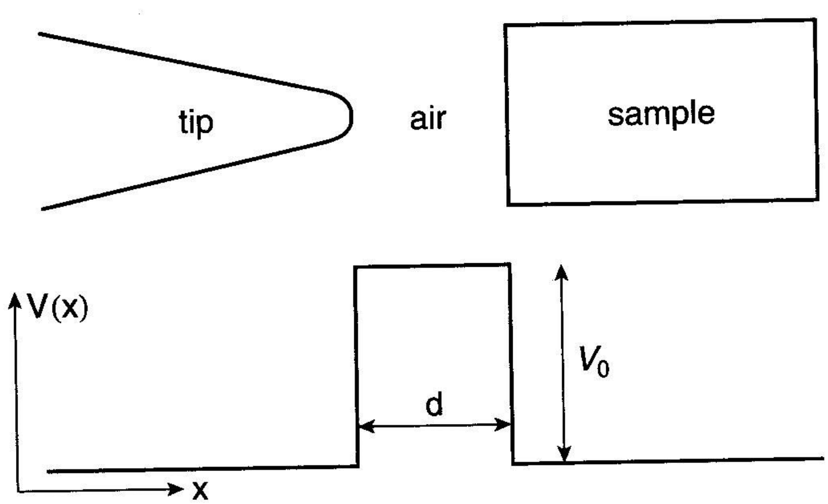

FIGURE 6.22 Schematic diagram of the scanning tunneling microscope, and the representation in terms of a potential energy diagram.

Figure 5.7: Sketch of a scanning/tunneling electron microscope

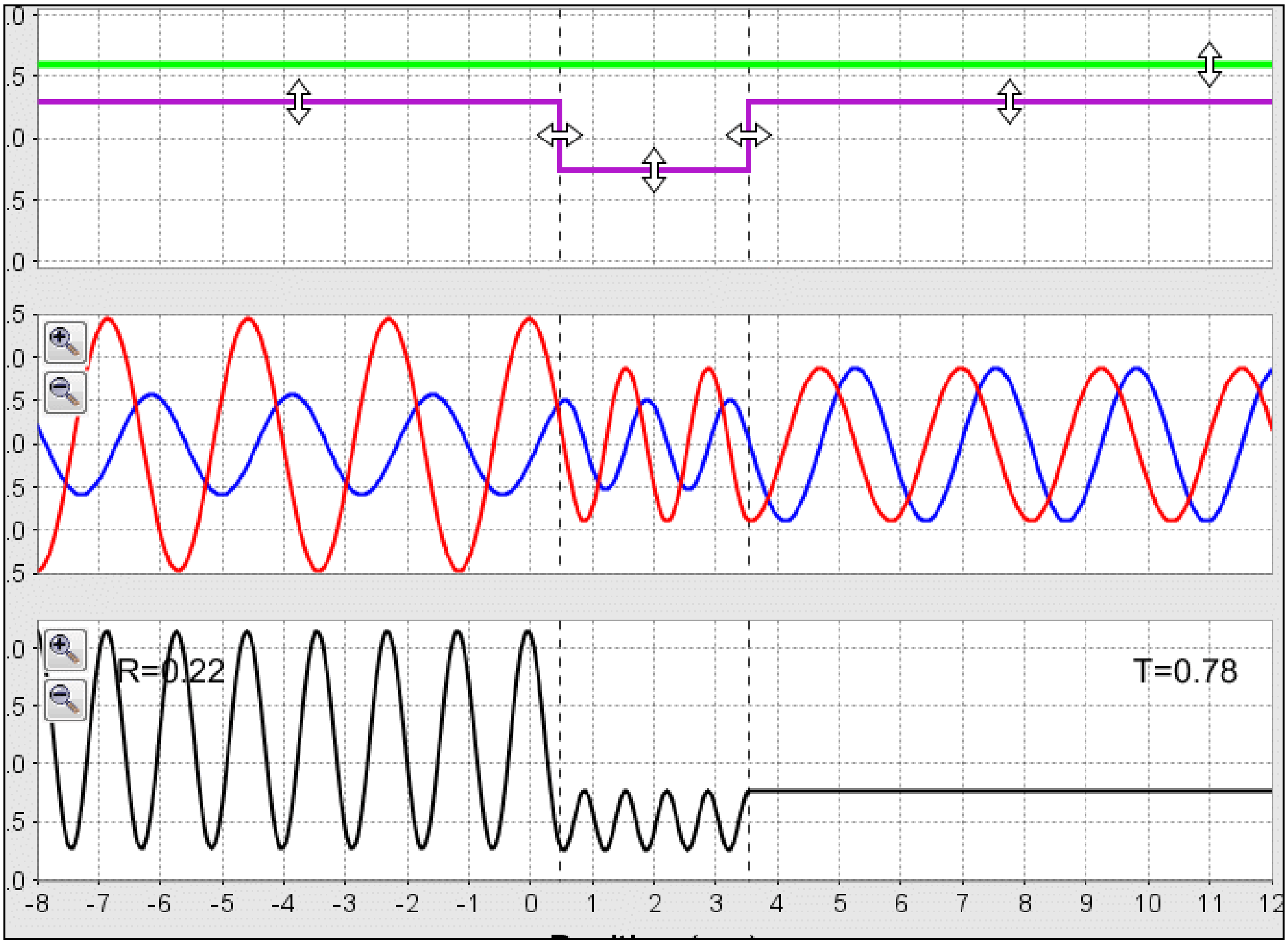

Figure 5.8: A stationary solution of a wave scattering off a square potential well

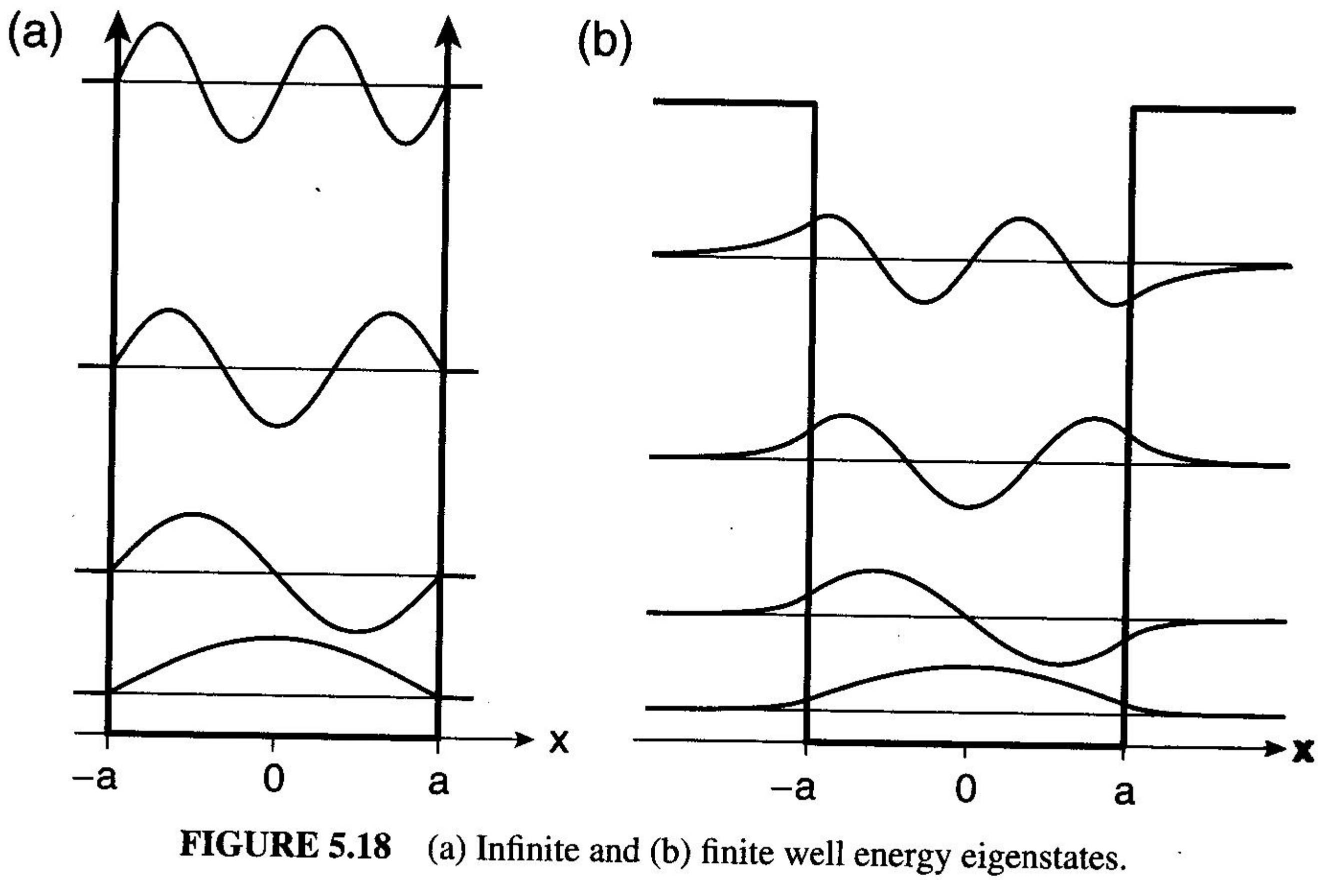

Figure 5.9: Bound states in a potential well.

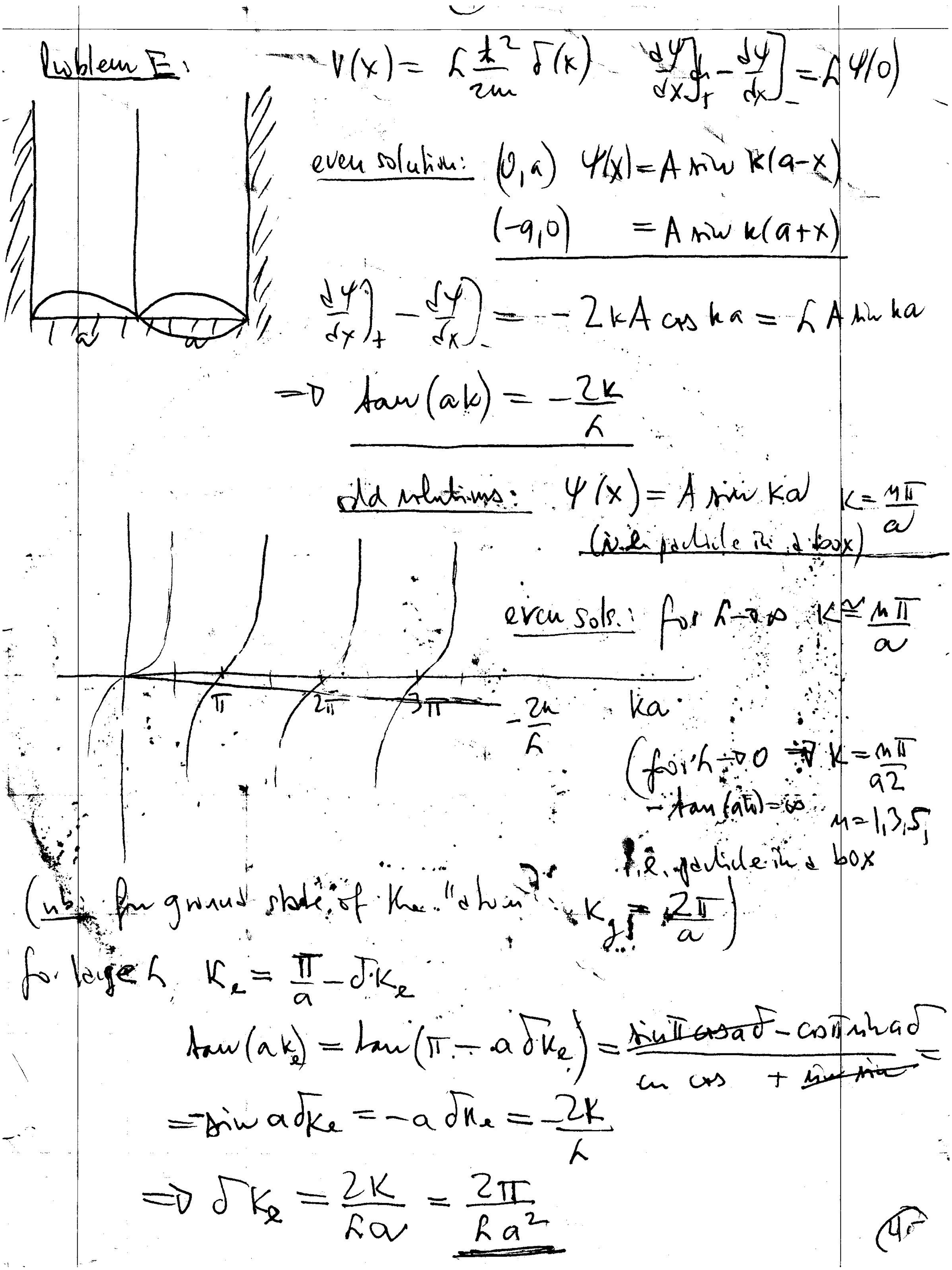

Figure 5.10: Bound states in a potential $V(x) = (\hbar^2/2m)\delta(x)$ for x between -a and +a, $V(x) = \infty$ outside. A simple (but analytically solvable!) model of a molecular ion.

Chapter 6

Quantum Physics in Hilbert Space

6.1 Hilbert Space

It so happens (this should be taken as an "experimental" fact) that the space of quantum-mechanical states is a Hilbert space: a vector space consisting of abstract vectors $|\psi>, |\phi>, |x>, |n>, \ldots$ with "reasonable" properties for addition and multiplication of vectors by complex numbers (i.e. commutative, distributive and associative laws, plus existence of a unique null vector).

In addition, a bilinear "inner product" (a generalization of the ordinary scalar product of two vectors) is defined, with

$$<\phi|\psi> = <\psi|\phi>^*$$

As we shall see, the "dual" vectors [1] are generalizations of complex conjugation.

The physics meaning of $<\phi|\psi>$ is the probability amplitude of finding system $|\psi>$ in state $|\phi>$. Important examples are $<x|\psi>$ is the probability amplitude of finding particle that was in state $|\psi>$ to be at position x. So $<x|\psi> = \psi(x)$ – our old friend, the wave function. Similarly, for a particle in a potential box, $<n|\psi>$ is the probability ψ_n of finding the particle in the n-th energy state, i.e. with energy E_n (by convention, the continuous variable is usually written as an argument, discrete variable as an index).

6.1.1 Operators and Observables

Operators in Hilbert space operate on vectors to produce different vectors:

$$A|\psi> = |\phi>$$

An operator can operate on a bra or on a ket, according to the definition

$$<\phi|(A|\psi>) \equiv (<\phi|A)|\psi> \equiv <\phi|A|\psi>$$

[1] Since the form $<\,|\,>$ looks like a bracket, Dirac applied his "physicist's sense of humor" and called the vector $<\,|$ a *bra* and the vector $|\,>$ a *ket*. The space of the bra's is said to be "dual" to the space of the kets. The power of Dirac notation comes from the ability to put the full definition of the state inside the $|\,>$, so you may have $|\psi>$ or $|\textit{ground state of the Hydrogen atom}>$ etc. A numerical, quantitative representation of the abstract Hilbert state vector $|\psi>$ may then be a complex function $\psi(x) = <x|\psi>$ etc.

The definition of operator $A^\dagger$ to be an Hermitian-adjoint to operator A is [2]

$$<\phi|A|\psi> = <\psi|A^\dagger|\phi>^*$$

and if $A = A^\dagger$ we say that the operator A is Hermitian. It is easy to see that the expectation values and the eigenvalues of a Hermitian operator are real (do it as HW). Therefore, physical observables are always represented by Hermitian operators.

It is easy to see that the eigenvectors of a Hermitian operator corresponding to different eigenvalues are mutually orthogonal (the case of degeneracy is discussed in the section on the Commutator):

$$A|\psi_1> = a_1|\psi_1>$$

$$<\psi_2|A = <\psi_2|a_2$$

$$<\psi_2|A|\psi_1> = a_1 <\psi_2|\psi_1>$$

$$<\psi_2|A|\psi_1> = a_2 <\psi_2|\psi_1>$$

$$\Rightarrow \qquad 0 = (a_1 - a_2) <\psi_2|\psi_1>$$

Examples:

- The set of all square-integrable functions is a Hilbert space, with the inner product defined as

  $$<f|g> = \int f^*(x)g(x)dx$$

  example of an operator would be $\hat{p} = -i\hbar\frac{\partial}{\partial x}$

  HW: prove that the operator $\hat{p}$ is Hermitian (hint: use integration by parts) (and appreciate, again, the importance of complex numbers in quantum physics).

- The set of n-dimensional complex vectors is a Hilbert space with the inner product

  $$<a|b> = \sum_{i=1}^{n} a_i^* b_i$$

  In this case, states (bra / kets) will be represented by n-dimensional row / column vectors, and operators will have the form of an $n \times n$ matrix.

  HW: show that an operator A is hermitian if $A_{ij} = A_{ji}^*$.

We will see how these (and other) examples appear as representations of the abstract Hilbert space of quantum-mechanical states.

[2] Unfortunately, many texts confuse this simple but subtle issue: Ohanian (an otherwise excellent text) writes $<\alpha|Q|\beta> = (<\alpha|Q^\dagger)|\beta>$ which is technically incorrect. Griffiths (eq. 3.15 - 3.17), Gasiorowicz (eq. 6-9) and many others write $<A\phi|\psi> = <\phi|A^\dagger|\psi>$ which is confusing at best: in Dirac notation, ψ is NOT a vector in Hilbert space - it is just a label, and an operator operating on a label does not make sense.

6.1.2 Quantum Physics in Hilbert Space Summarized

Here is an (informal) summary of the formal postulates of Quantum Mechanics: [3]

I. States of physical systems are represented by vectors in Hilbert space. Any linear combination (with complex coefficients) of possible states is a possible state. This is the Principle of Superposition (which is due to the linearity of the Schrodinger equation), and it leads to most of the quantum-mechanical conundrums.

II. The time development of a state is given by the Schrodinger equation

$$i\hbar \frac{d|\psi>}{dt} = H|\psi>$$

where H is the Hamiltonian (operator of energy) of the system.
Note that - in contrast to the Newton's law - this is a first-order equation.
Note also that time t appears, but position x does not - "existence happens in the Hilbert space". In other words, the non-relativistic quantum mechanics is non-local from the very start.

III. The probability that if we prepare the system in state $|\psi>$ we will find it in state $|\phi>$ is

$$P = |<\phi|\psi>|^2$$

where $<\phi|\psi>$ is the "probability amplitude".

IV. Any observable A is associated with a Hermitian operator A, and all possible outcomes of a measurement of A are the eigenvalues of A. After the measurement, the system will be in the corresponding eigenstate:

$$A|\psi_a> = a|\psi_a>$$

Va. The set of eigenvectors of a Hermitian operator is complete: an arbitrary state $|\phi>$ can be expressed as a linear combination (a sum or an integral - see Section 3a and 3b below):

$$|\phi> = \sum_a c_a|\psi_a>$$

Vb. The set of eigenvectors is (or can be made) orthonormal:

$$<m|n> = \delta_{mn} \qquad <q|q'> = \delta(q-q')$$

for discrete or continuous spectrum, respectively.

[3] In the following, we omit the "hat" above the operator symbol when there is no danger of confusion, so instead of $\hat{A}$ we will simply use A.

6.1.3 Hilbert Space Representations

When we choose a "basis", i.e. a **complete** set of **orthonormal** states (a discrete set of $|m>$, or a continuous "set" of $|x>$), we obtain a particular representation of the abstract Hilbert space.

a) discrete case: the orthonormality is expressed by $< m|n >= \delta_{mn}$. Completeness means that any state $|\psi>$ can be expressed as a linear combination of the base states $|n>$

$$|\psi >= \sum_n c_n|n >$$

where the complex coefficients c_n can be easily determined by making inner product of this equation with $< m|$, and using the orthonormality:

$$< m|\psi >=< m|\sum_n c_n|n >= \sum c_n\delta_{mn} = c_m$$

This means that the expansion can be written as

$$|\psi >= \sum_n < n|\psi > |n >= (\sum_n |n >< n|)|\psi >$$

Therefore, the operator

$$I \equiv \sum |n >< n|$$

is an identity operator, and can be inserted in expressions for the inner product or for the expectation value, in the eigen-equation etc. Consequently, in the discrete case, states are **represented** by state vectors

$$c_m =< m|\psi >$$

while operators are represented by matrices [4]

$$A_{mn} =< m|A|n >$$

and eigen-equations reduce to matrix equations

$$\sum_n A_{mn}c_n = ac_m$$

This is the "matrix" (Heisenberg) formulation of Quantum Mechanics (compared to "wave" (Schrödinger) formulation. It will be very useful for description of **spin**.

[4] Recall that the first index (i) in a matrix element A_{ij} represents the row, and the second index (j) represents the column. So for example, a multiplication of two matrices C = AB

$$C_{ij} = \sum_k A_{ik}B_{kj}$$

is verbalized (do it!) as follows: "the element at the intersection of i-th row and j-th column is the scalar product of i-th row of the first matrix with the j-th column of the second matrix".

b) In the continuous case, the orthonormality condition is $< q|q' >= \delta(q-q')$. Completeness means that any state $|\psi >$ can be expressed as a linear combination of the base states $|q >$:

$$|\psi >= \int dq\ c(q)|q >$$

where the complex coefficient $c(q')$ can be determined by making inner product of this equation with $< q'|$ and using the orthonormality:

$$< q'|\psi >=< q'| \int dq\ c(q)|q >= \int dq\ c(q) < q'|q >= \int dq\ c(q)\delta(q-q') = c(q')$$

This means that the expansion can be written as

$$|\psi >= \int dq < q|\psi > |q >= (\int dq|q >< q|)|\psi >$$

Therefore, the operator

$$I \equiv \int dq|q >< q|$$

is an identity operator, and can be inserted in inner products, expectation values, eigen-equations etc.
States are represented by **state functions**

$$\psi(x,t) =< x|\psi >=< \psi|x >^*$$

or $\psi(p,t) =< p|\psi >$ etc., i.e. any given state $|\psi >$ can have many equivalent "representations" $< x|\psi >, < p|\psi >$,...). Operators are represented by (uncountably infinite-dimensional) "matrices" $A(x,x') =< x|A|x' >$.
It is easy to se that

$$< x'|\hat{x}|x'' >= x'\delta(x'-x'')$$

so that $\hat{x} = x$. Example:

$$< x >= \int \psi^*(x)x\psi(x)dx$$

It is somewhat more difficult (we will skip the proof) to show that, in the x-representation, the momentum operator is $\hat{p} = -i\hbar\partial/\partial x$.

6.1.4 Relations between different representations:

The transformations between different representations are accomplished by using the resolution of the identity again. Notice how the familiar notions such as coordinate system rotation, Fourier transform or a Fourier series, are all just a special case of the Hilbert space representation change:

$$\psi(x) =< x|\psi >= \int dp < x|p >< p|\psi >= \int dp \; e^{ipx/\hbar}\phi(p)$$

$$\psi(x) =< x|\psi >= \sum_n < x|n >< n|\psi >= \sum_n \xi_n(x)\psi_n$$

$$\psi_n =< n|\psi >= \int dx < n|x >< x|\psi >= \int dx \; \xi_n^*(x)\psi(x)$$

$$\psi_n =< n|\psi >= \sum_{m'} < n|m' >< m'|\psi >= \sum_{m'} c_{nm'}\psi_{m'}$$

(note: the meaning of the terms in the last column can be seen from the middle column: the first example is a transformation from a continuous base to a different continuous base (in this case specifically $p \to x$), second example is discrete $\to$ continuous, third example is continuous $\to$ discrete, and last is discrete $\to$ discrete. In the last example, n labels one set of the base states $\{n\}$, and m' labels another set of base states $\{m'\}$.

6.1.5 Expectation value:

Show, as HW, that the expectation values are

$$< A >_\psi \; = \; < \psi|A|\psi > \; = \sum a_i|c_i|^2 = \int dq \; a(q)|c(q)|^2$$

where a_i is the eigenvalue corresponding to the i-th eigenstate of A in the discrete case, $a(q)$ is the eigenvalue corresponding to the "q-th" eigenstate of A in the continuous case, and c_i or $c(q)$ are the corresponding probability amplitudes.

6.2 The Great Commutator

The commutator of two operators

$$[A, B] \equiv AB - BA$$

plays a fundamental role in Quantum Physics. The following four subsections explain this role in some detail:

6.2.1 Structure of the commutator is independent of representation

It is easy to see that the structure of the commutation relation is the same in any representation: if in the Hilbert space $[\hat{A}, \hat{B}] = \hat{C}$ then in any representation $[A, B] = C$. In particular, if $[\hat{A}, \hat{B}] = c$ where c = complex number (i.e. the operator $c * \hat{I}$), then $[A, B] = c$ in any representation (recall the example of $[\hat{x}, \hat{p}]$ in the x- and p-representations).

6.2.2 General Heisenberg Uncertainty relation III

Define the uncertainty of A by

$$\delta A = \sqrt{< (a- < a >)^2} = \sqrt{< A^2 > - < A >^2}$$

Then define operators $U \equiv A- < A >$ and $V \equiv B- < B >$ and convince yourself that

$$\delta A = \sqrt{< U^2 >} \qquad \delta B = \sqrt{< V^2 >} \qquad [U, V] = [A, B]$$

Now investigate, as HW, the behavior of the quantity

$$I(\lambda) \equiv < U + i\lambda V | U + i\lambda V >$$

for real values of λ. Obviously, $I(\lambda) \geq 0$ for any value of λ. Show that $I(\lambda)$ is smallest (but of course still non-negative) for

$$\lambda = -i \frac{(< [U, V] >)^2}{2 < V^2 >}$$

(and pause for a moment to show that this indeed is a real number for any two Hermitian operators U and V.) Then plug it into the definition of $I(\lambda)$ and show that the grand result is:

For any two Hermitian operators A and B, in any state $| \psi >$:

$$\delta A . \delta B \ \geq \ \frac{1}{2} | < \psi \mid [A, B] \mid \psi > |$$

a) if A and B do not commute, this gives the most general form of the uncertainty relation (this is of course the famous Heisenberg Uncertainty Relation). Note the precise meaning: given an ensemble of many identical copies of a quantum system, you measure A on some of them, and B on the others. The resulting distributions of measured values a and b obey the Heisenberg Inequality. Note that this is a different interpretation than that of professor Heisenberg himself (he considered performing both measurements on the same event, and the first measurement disturbed the system ...).

b) if A and B do commute, this expression says that the corresponding observables can be measured simultaneously. This corresponds to the fact that commuting operators have common eigen-functions (see next section).

6.2.3 Maximum set of commuting observables

Commuting operators have common eigen-functions:

Apply B to both sides of $A|\psi>= a|\psi>$, and commute A with B to obtain

$$AB|\psi>= aB|\psi>$$

This means that the state $|\phi>= B|\psi>$ is an eigenstate of A, with eigenvalue a.

a) the **non-degenerate** case: there is only one independent eigenstate of A corresponding to eigenvalue a. Therefore, $|\phi>$ must be proportional to $|\psi>$, i.e. $|\phi>= B|\psi>= b|\psi>$, i.e. $|\psi>$ is also an eigenstate of B.

b) the **degenerate** case: consider two independent eigenstates of A corresponding to the same eigenvalue. Dropping the hats and brackets to save some typing, we have:

$$A\psi_1 = a\psi_1 \text{ and } A\psi_2 = a\psi_2$$

As in case a), the states $B\psi_1$ and $B\psi_2$ are eigenstates of A, and can therefore be expressed as some linear combinations of the independent eigenstates ψ_1 and ψ_2 of A:

$$B\psi_1 = \alpha_1\psi_1 + \beta_1\psi_2 \text{ and } B\psi_2 = \alpha_2\psi_1 + \beta_2\psi_2$$

Is there $\phi = \psi_1 + \lambda\psi_2$ such that $B\phi = b\phi$? By equating the coefficients multiplying ψ_1 and ψ_2, you should obtain a quadratic equation for λ. There are therefore **two** solutions to the eigenequation for B, each with different eigenvalue b (but the same eigenvalue a of A). The two eigenstates ϕ are therefore orthogonal.

In the general case, this procedure is repeated until all degeneracy is removed. A maximum set of mutually commuting operators is called a **complete set**, and its eigenvalues fully specify a quantum-mechanical state. (Simplest example: the two-fold degeneracy of the energy of free particle, removed by specifying of eigenvalue of momentum (do as HW).)

6.2.4 Time-dependence of the expectation values and transition to classical

The Commutator governs the time-dependence of the expectation values:

It is easy to show (HW) from the Schrödinger equation that

$$\frac{d<A>}{dt} =< \frac{\partial A}{\partial t} > + \frac{i}{\hbar} < [H, A] >$$

In particular, this means that if an observable, not explicitly dependent on time, commutes with the Hamiltonian, then its expectation value is conserved, **in any state**. This is different from the notion of stationary state (an eigenstate of the Hamiltonian), where the expectation value is conserved for **any observable.**

6.2.5 Schrödinger equation and Newton's law

Using the above equation it is easy to show (HW) that

$$\frac{d < x >}{dt} = \frac{< p >}{m} \quad \text{and} \quad \frac{d < p >}{dt} = - < \frac{dV}{dx} > = < F(x) >$$

This is very similar to the Newton's law $dp/dt = F$ but we are not quite there yet. For the true correspondence we need $< F(x) >= F(< x >)$ and this is the subject of the **Ehrenfest principle:**

For potentials that are slowly varying over the region where the wave-function is appreciable:

$$- < \frac{dV(x)}{dx} >= -\frac{dV(< x >)}{d < x >} = F(< x >)$$

proof:

$$< F(x) > = < F(< x >) + (x- < x >)F'(< x >) + \frac{1}{2}(x- < x >)^2 F''(< x >) + ... > \cong$$

$$\cong < F(< x >)+ < x- < x >> F'(< x >) \;\; = \;\; F(< x >)$$

and we get

$$m\frac{d^2 < x >}{dt^2} = F(< x >)$$

in words: the center of a quantum wave-packet moves according to the Newton's law (even in purely quantum-mechanical regime !). Note that the restriction to slowly varying potentials is essential: recall the reflection from a potential step!

6.2.6 Does Quantum mechanics Satisfy the Equivalence Principle?

Note that the Schrödinger equation for a particle in gravitational field

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + mg\psi$$

contains an explicit mass dependence which does not cancel out. Although the motion of the center of mass is independent of m:

$$\frac{d^2 < x >}{dt^2} = g$$

one might expect a mass dependence to turn up in a sufficiently subtle experiment. This is indeed the case: consider the setup where a neutron can go from A to D either via B or via C (see Figure). It is easy to calculate the phase difference $\Delta\phi = \phi_{ABD} - \phi_{ACD}$, as a function of the tilt-angle δ. Since the phase difference on segments CA and BD is equal, it is sufficient to compare segments AB and CD. From energy conservation

$$E = p^2/2m = p'^2/2m + mgl_2\text{sin}\delta$$

one gets

$$\Delta\phi = l_1\Delta k \cong l_1(k'^2 - k^2)/2k = -m^2 g l_1 l_2 \lambda \text{sin}\delta/2\pi\hbar^2$$

The same result can be obtained from $\Delta\phi = \omega\Delta t$.
Remarkably, this effect has indeed been observed using a neutron interferometer.

6.2.7 Conservation laws in Quantum Mechanics

Recall that if an operator A, not explicitly dependent on time, commutes with the Hamiltonian, its expectation values are conserved. In particular, if

$$A\psi(x,0) = a\psi(x,0) \;\; \text{then} \;\; A\psi(x,t) = a\psi(x,t).$$

This can be nicely illustrated with the help of the formal solution of the Schrödinger equation with a time-independent Hamiltonian:

$$|\psi(t >= e^{-iHt/\hbar}|\psi(0) >$$

This gives:

$$< \psi(t)|A|\psi(t) > = < \psi(0)|e^{iHt/\hbar} A e^{-iHt/\hbar}|\psi(0) > = < \psi(0)|A|\psi(0) > .$$

6.2.8 Conservation of parity from Symmetry of potential

The implication of an operator commuting with the Hamiltonian on the structure of the Hamiltonian is best explained on the example of the parity operator:

$$0 = [H,P]\psi(x) = [V(x),P]\psi(x) = V(x)P\psi(x) - PV(x)\psi(x) = V(x)\psi(-x) - V(-x)\psi(-x)$$

Therefore, for parity to be conserved, the potential must be symmetric ($V(x) = V(-x)$).

6.2.9 Conservation of momentum from Homogeneity of space

In general, each symmetry (invariance in respect to a transformation) has a "generator" which corresponds to a conserved observable. As an important example, consider the translational invariance (i.e. homogeneity of space). The generator of a translation in space is the momentum operator:

infinitesimal translation:

$$\psi(x+\epsilon) = \psi(x) + \epsilon\frac{df}{dx} = T(\epsilon)\psi$$

$$\text{where} \quad T(\epsilon) = 1 + \epsilon\frac{d}{dx} = 1 + \frac{i}{\hbar}p\epsilon$$

finite translations:

$$\psi(x+a) = T(a)\psi(x) \quad \text{where} \quad T(a) = \lim_{n\to\infty}(1 + \frac{i}{\hbar}\frac{a}{n}p)^n = e^{ipa/\hbar}$$

For Schrödinger equation to be invariant in respect to translations:

$$T(i\hbar\frac{\partial\psi}{\partial t}) \;=\; T(H\psi) \quad \Rightarrow \quad i\hbar\frac{\partial(T\psi)}{\partial t} = H(T\psi)$$

$\hat{T}$ must commute with $\hat{H}$, i.e. $\hat{p}$ must commute with $\hat{H}$, i.e. momentum will be conserved.

6.2.10 Conservation of Energy from Homogeneity of time

You can now see that the meaning of the Schrödinger equation is: "generator of the translations in time is the Hamiltonian." This is explicitly seen comparing the expression for T with the formal solution of the Schrödinger equation

$$\psi(x,t) = U(t)\psi(x,0) \quad \text{where} \quad U(t) = e^{-itH/h}$$

Homogeneity of time thus leads to the conservation of energy. Similarly, invariance in respect to rotations (i.e. isotropy of space) will lead us to the concept of angular momentum and to its conservation.

6.3 Simple Harmonic Oscillator

This section is of great practical as well as theoretical and pedagogical importance. The SHO potential

$$V(x) \ \sim \ x^2 + p^2$$

occurs in a wide variety of physics situations, either directly, or as an approximation close to a local minimum. The familiarity with the Hilbert space method of the SHO solution is an absolute necessity for student to master dealing with commutation relations, and it is a great precursor to a very similar treatment of the angular mpmentum. Therefore the whole section is assigned as HW: students will be expected to fill in the missing steps and missing constants (such as $m, \omega, \hbar$ etc.) and a problem testing your understanding may well come in the 2nd midterm or in the Final Exam. Everything is treated in great detail in Griffiths section 2.3 - 2.3.1, as well as in Pnini section 5.4 and Solved Problems 5.8-5.10.

6.3.1 The ladder operators

The procedure starts with switching from operators x and p to the new operators of the form [5]

$$a_\pm \sim x \mp ip$$

These operators do not represent any physical quantity as they are not Hermitian ($a_+^\dagger = a_- \neq a_+$). Instead, we use them, and the inverse relationship

$$x \sim \ (a_- + a_+) \qquad p \sim \ (a_- - a_+)$$

to obtain the expressions for the commutator and for the Hamiltonian:

$$[a_-, a_+] = 1 \qquad\qquad H = \hbar\omega(a_\pm a_\mp \pm \frac{1}{2})$$

Assuming that $|E>$ is an eigenfunction of the Hamiltonian with the eigenvalue E, it is then easy and in fact extremely elegant to show that

[5] Note that Pnini (and many other texts) denote Griffiths' operators a_- and a_+ by a and $a^\dagger$, respectively

$$H(a_+|E>) = \hbar\omega(a_+a_-a_+ + \frac{1}{2}\ a_+)E >= \hbar\omega a + (a_+a_- + 1 + \frac{1}{2})|E >= a_+(H + \hbar\omega)|E >=$$

$$= (E + \hbar\omega)(|a_+|E>)$$

This means that the state $a_+E >$ is an eigenstate of H with eigenvalue increased by the amount $\hbar\omega$ (=hf !): $a_+|E >\sim |E + \hbar\omega >$
Similarly, the operator a_- decreases E to $E - \hbar\omega$. We then we apply the lowering operator a_- repeatedly, until we reach the ground state that cannot be lowered, i.e.

$$a_-|E_0 >= 0$$

and the actual value of the ground state energy is immediately obtained from

$$H|E_0 >= \hbar\omega(a_+a_- + \frac{1}{2} >= \frac{1}{2}\ \hbar\omega|E_0 >$$

So there you have it: we have obtained (in Hilbert space !) the spectrum of SHO as equidistant energy levels with spacing hf sitting on the "zero-point energy" $E_0 = \frac{1}{2}hf >$ (due, in final analysis, to the Heisenberg Uncertainty Principle). And then all higher sates are obtained by repeated application of the raising operator a_+ on $|E_0 >$.

Going from Hilbert space to the coordinate representation, the equation $a_-|0 >$ becomes a simple differential equation

$$a_-\psi_0(x)\ \sim\ (x + ip)\psi_0(x) = 0$$

with the immediate solution

$$\psi_0(x) \sim e^{-x^2}$$

It can be verified by direct integration of $|\psi_1|^2$ (see Griffiths Example 2.4) that the normalization coefficient for ψ_1 is 1.0, i.e. in Hilbert space, changing notation from $|E_n >$ to $|n >$

$$a_+|0 >= |1 >$$

The normalization for higher states is then obtained from realizing that

$$a_+a_-|n >= n|n > \qquad a_-a_+|n >= (n + 1)|n >$$

so that if $< n|n >= 1$ and $< n + 1|n + 1 >= c$ then

$$< n|a_-a_+|n >=< n|(a_-a_+|n >) = (n + 1) = (< n|a_-)(a_+|n >) = c^2$$

so that

$$a_+|n >= \sqrt{n + 1}|n + 1 > \qquad a_-|n >= \sqrt{n}|n - 1 >$$

It is fun to watch how the repeated application of the raising operator then produces all the eigenstates

$|n >= \frac{1}{\sqrt{n!}}(a_+)^n|0 >$ corresponding to $E_n = (n + \frac{1}{2})\hbar\omega$

6.3.2 The wave functions

Going back to the coordinate space: all eigenstates $\psi_n(x)$ inherit the Gaussian exponential factor from $\psi_0(x)$, corresponding to the penetration into the left and right forbidden regions, multiplied by an n-th degree polynomial obtained by the repeated addition ox x and differentiation; physically this corresponds to the "wiggles" required by Dr. deBroglie as the particle moves in the allowed region between the turning points. The polynomials are important in many physics applications, and are called the "Hermite polynomials". Figure **??** shows several lowest wavefunctions, as well as a high-n wavefunction to illustrate the transition to the classical regime. Note that even the large-n state will not oscillate - this needs an addition of at least two states of different energy. Note also that a wave packet consisting of many states (e.g. n=91, 92, ...109, 100) will oscillate at the frequency corresponding to the energy difference of two consecutive states!

6.3.3 Vector/matrix representation

Finally, it is interesting to change from the coordinate representation to the energy representation , where states are represented by the ("ordinary") vectors [6]:

$$|0 >\rightarrow (1,0,0,0,....)$$

$$|1 >\rightarrow (0,1,0,0,....)$$

$$|2 >\rightarrow (0,0,1,0,....)$$

and so on, and operators are represented by matrices, such as

$$\hat{x} \rightarrow x_{nm} =< n|x|m >\sim< n|(a_+ + a_-)|m >$$

Such representation will be crucial when we discuss the states with half-integer angular momentum.

[6] I am typesetting these a row-vectors, but they really should be vertical column vectors ...

Chapter 7

Angular Momentum

7.1 Introduction

The operator of angular momentum is a straightforward generalization of the classical expression:

$$\hat{\vec{L}} = \hat{\vec{r}} \times \hat{\vec{p}}$$

Its components, using the Levi Civita symbol [1] are

$$\hat{L}_i = \sum_j \sum_k \epsilon_{ijk} \hat{r}_j \; \hat{p}_k$$

(HW: use this to write explicit expressions for the three components)

We will also need the operator for the square of the magnitude of the angular momentum. Omitting the hats, this is

$$L^2 = L_x^2 + L_y^2 + L_z^2$$

We will have to use the above definition expressed in spherical coordinates [2] (Griff. Fig. 4.1 and eqs. 4.123 - 4.132). Note how much more complex these equations (and the expression for the Laplacian - Griff. eq. 4.13) are in spherical coordinates than in the Cartesian coordinates. The exception is eq. 4.129:

$$L_z = -i\hbar \frac{\partial}{\partial \phi}$$

HW: Derive this equation, and ponder its connection to the earlier one dimensional definition

$$p = -i\hbar \frac{\partial}{\partial x}$$

[1] defined as 1) $\epsilon_{123} = +1$; same for the two cyclic permutations of indices ($\epsilon_{312} = \epsilon_{231} = +1$) 2) ϵ_{ijk} changes sign on an exchange of two indices It follows that the "anti-cyclic permutations $\epsilon_{321} = \epsilon_{132} = \epsilon_{213} = -1$ and all other $\epsilon_{ijk} = 0$ (i.e. those with at least one pair of equal indices). The full power of this symbol will become apparent in your $E\&M$ course.

[2] Note that $x = r\sin\theta\cos\phi \quad y = r\sin\theta\sin\phi \quad z = r\cos\theta$ and $d\Omega = r^2\sin\theta \; dr \; d\theta \; d\phi$

7.1.1 Commutation properties

It is easy to show that the three components of the operator $\hat{\vec{L}}$do not commute with each other, but each of them does commute with L^2:

$$[L_i, L_j] = i\hbar\epsilon_{ijk}\ L_k \qquad\qquad [L^2, L_i] = 0$$

Therefore, we can choose one component (traditionally L_z) and find the common eigenfunctions with L^2:

$$L^2|\lambda, \mu >= \lambda|\lambda, \mu >$$

$$L_z|\lambda, \mu >= \mu|\lambda, \mu >$$

7.1.2 The ladder operators, revisited

This proceeds, remarkably enough, along the lines of Simple Harmonic Oscillator. Defining $L_\pm = L_x \pm iL_y$ we get

$$L_z(L_+|\lambda, \mu >= (\mu + \hbar)L_+|\lambda, \mu >$$

This means that the state $L_+|\lambda, \mu >$ corresponds, up to a normalization constant, to the state $|\lambda, \mu+\hbar >$. But this raising of μ must stop when we reach a certain value μ_{max}, because a projection of a quantity cannot exceed the quantity itself, and therefore

$$L_+|\lambda, \mu_{max} >= 0$$

This, and subsequent use of L_-, leads to the explicit construction of all states. Changing the labeling of the states from $|\lambda, \mu >$ to $|l, m >$, the final result is

$$L^2|l, m >= l(l + 1)\hbar^2|l, m >$$

$$L_z|l, m >= m\hbar|l, m >$$

where $-l \leq m \leq l$ with unit distance between the consecutive values of m.

7.1.3 The two families of angular momentum states

An obvious solution is a family of integer values on m:
l = 0, m = 0
l = 1, m = -1,0,1
l = 2, m = -2,-1,0,1,2
etc.
As in Simple Harmonic Oscillator, again, the explicit representations by functions $Y_l^m(\theta, \phi)$ are determined from $L_+Y_l^l = 0$, and $Y_l^{m-1} \sim L_-Y_l^m$. These so called "spherical harmonics" are easy to obtain if you are patient - they get complicated quite quickly - see Griffiths Table 4.3, and Figures.

The second, less obvious family of solutions is for half-integer values of l:

$l = \frac{1}{2}, m = -\frac{1}{2}, \frac{1}{2}$

$l = \frac{3}{2}, m = -\frac{3}{2}, -\frac{1}{2}, \frac{1}{2}, \frac{3}{2}$
etc

Remarkably, these states cannot be due to any orbital motion [3] . So the family of solutions of the commutation relations is larger than the operator $\hat{\vec{r}} \times \hat{\vec{p}}$ that was at the origin of the commutators. And even more remarkably, these states indeed exists in Nature - in fact you are made of them (protons, neutrons and electrons all have "inherent angular momentum" $\frac{1}{2}$)!

7.1.4 Summary of the notation

Traditionally, we distinguish three kinds of angular momentum by using symbols L, S and J:

L^2, L_z (with eigenvalues labeled by l, m) denote "orbital angular momentum". The values of l are restricted to integers 0,1,2,...
S^2, S_z (with eigenvalues labeled by s, m) denote "spin" - the angular momentum in the rest-frame of the particle
J^2, J_z (with eigenvalues labeled by j, m) denote generic angular momentum.

Spin (or generic angular momentum) may be integer or half-integer (of orbital nature, of inherent (quantum) nature, or hybrid).

Most importantly, several identical particles of integer spin ("bosons") obey the "Bose-Einstein statistics": the wave function is symmetrical upon any exchange. On the other hand, several identical particles of half-integer spin ("fermions") obey the "Fermi-Dirac statistics": the wave function is anti-symmetric upon any exchange, i.e. changes sign. Therefore, two (or more) identical fermions cannot be in the same quantum state. As we shall see, this (the "Pauli exclusion principle") is the foundation of the periodic table, and in fact foundation of all atomic physics.

7.1.5 Addition of angular momenta

We will need to be able to deal with several angular momenta in the same system. Classically, this is just a sum of the angular momentum vectors of the individual components (such as for example Moon's spin around its axis, combined with its orbital momentum as it goes around the Earth). As you might expect, in QM it gets a little more tricky: addition of angular states $|j_1, m_1>$ and $|j_2, m_2>$ results in one of the states $|j, m>$ with $m = m_1 + m_2$ and $|j_1 - j_2| \leq j \leq (j_1 + j_2)$. The full treatment is quite tricky, but fortunately in this class we will only need to analyze the simplest case of $j_1 = j_2 = \frac{1}{2}$. This enables us to use a very simple notation: we will need the relation between:

the representation using $|j, m>$ (four states: $|1, 1>, |1, -1>, |1, 0>$ and $|0, 0>$)
and

[3] An elegant way to see that is to show that $L_- Y_{\frac{1}{2}}^{\frac{1}{2}} \neq Y_{\frac{1}{2}}^{-\frac{1}{2}}$. HW: do this, or at least think about how would you do it.

the different but equivalent representation using $|m_1, m_2>$ (four states: $|\frac{1}{2}, \frac{1}{2}>, |-\frac{1}{2}, \frac{1}{2}>$, $|\frac{1}{2}, -\frac{1}{2}>$ and $|-\frac{1}{2}, -\frac{1}{2}>$)

The first two states are easy: clearly $|1,1>=|\frac{1}{2}, \frac{1}{2}>$ and $|1,-1>=|-\frac{1}{2}, -\frac{1}{2}>$
The state $|1,0>$ can be obtained by applying the lowering operator J_- on the state $|1,1>$. Using the action of J_- derived above[4], we obtain

$$|1,0>=\frac{|\frac{1}{2}, -\frac{1}{2}>+|-\frac{1}{2}, \frac{1}{2}>}{\sqrt{2}}$$

The last state is

$$|0,0>=a|\frac{1}{2}, -\frac{1}{2}>+b|-\frac{1}{2}, \frac{1}{2}>$$

and the values of the coefficients a and b are obtained from orthonormality:

$$<1,0|0,0>=0=(a+b)\sqrt{2} \qquad <0,0|0,0>=1=a^2+b^2$$

yielding

$$|0,0>=\frac{|\frac{1}{2}, -\frac{1}{2}>-|-\frac{1}{2}, \frac{1}{2}>}{\sqrt{2}}$$

The remarkable properties of this state will lead us, in the Grand Finale, to the famous Bell Inequality.

7.1.6 Angular Momentum as the Generator of Rotations

Upon an infinitesimal rotation of the coordinate system around the z-axis by angle ϵ, a function f transforms as

$$f'(x,y,z)=f(x-\epsilon y, y+\epsilon x, z)$$

$$=f(x,y,z)-\epsilon y\frac{\partial f}{\partial x}+\epsilon x\frac{\partial f}{\partial y}=(1+i\epsilon L_z/\hbar)f(x,y,z)=D_z(\epsilon)f(x,y,z)$$

A finite rotation is then obtained by the operator

$$D_z(\phi)=\lim_{n\to\infty}(D_z(\phi/n))^n=e^{iL_z\phi/\hbar}$$

$$\Rightarrow D_z(\phi)\,|jm\rangle=e^{im\phi}\,|jm\rangle$$

This equation will be your main tool in the homework ....

Notes

- The above results use the Taylor expansion of $f(x-\epsilon, y+\epsilon, z)$ around (x,y,z), and the binomial expansion of an exponential

-The similarity of the operator of translation in the z-direction

$$D_z(a)=e^{ip_z a/\hbar}$$

[4]Note that when applying J_- on the right-hand side, you must apply it only the first particle, then only on the second particle, and add the results.

is not accidental: recall that in spherical coordinates $L_z = -i\hbar\partial/\partial\phi$.
-We see that the operator L_z is a 'generator of rotations around the z-axis'. This turns out to be independent of the particular representation, i.e. it is true in the Hilbert space. It is also valid for situations in which angular momentum cannot be described in a coordinate representation at all, i.e. for 'spin'.
-To get the 'active rotation' (i.e. rotation of the object), change ϕ to $-\phi$.
-The physics consequences: if H is invarient with respect to rotations around z $\Rightarrow [H, D_z] = 0 \Rightarrow [H, L_z] = 0 \Rightarrow L_z$ is conserved. This is the same reason which leads to the conservation of $\hat{\vec{p}}$ if H is invariant with respect to translations.
-The same results are obviously obtained for the x- and y-projections. An arbitrary rotation is obtained by a suitable combination of rotations around around different axes, and an invariance of the Hamiltonian with respect to such a rotation leads to the conservation of the angular momentum $\hat{\vec{J}}$.
-Now you can see that two rotations do not, in general, commute because their generators do not commute, which is due to the fact that $[L_z, L_y] \neq 0$. (In classical physics, rotations are represented by matrices, and we know matrices in general do not commute).
- Consider two coordinate systems with axes z and z'. Obviously, either $|jm\rangle$ or $|jm'\rangle$ form complete sets of orthonormal states. Therefore

$$|jm'\rangle = \sum_m |jm\rangle \langle jm|jm'\rangle = \sum_m c_{mm'} |jm\rangle$$

and

$$|jm\rangle = \sum_{m'} |jm'\rangle \langle jm'|jm\rangle = \sum_m^{\prime} c_{m'm} |jm'\rangle$$

where the coefficients c_{ij} have the usual probability interpretation.
Note that the above transformation between two bases in Hilbert space is analogous to the relation between two mutually rotated bases in an ordinary vector space. Recall another example of such a transformation – the Fourier transform.
Note also that it is easy (and instructive) to transform the matrix representing an operator to the new basis.

7.1.7 Half-integer angular momentum

The angular momentum operator $\hat{J}$ cannot be represented as $\hat{r} \times \hat{p}$ in the case of half-integer j. The see this, look at the action of raising and lowering operators $J_\pm = J_x \pm iJ_y$ in the spherical coordinate representation in which

$$|jm\rangle \to Y_{jm}(\theta, \phi)$$

and

$$J_\pm \to \hbar e^{\pm i\phi}(\pm\frac{\partial}{\partial\theta} + i\cot\theta\frac{\partial}{\partial\phi})$$

The equations

$$J_\pm Y_{j\pm j} = 0$$

and

$$J_z Y_{j\pm j} = \pm j\hbar Y_{j\pm j}$$

can easily be shown to have the solution

$$Y_{j\pm j}(\theta, \phi) \sim e^{\pm ij\phi} \sin^j \theta$$

You should verify that $\hat{J}^2 Y_{j\pm j} = j(j+1)\hbar^2 Y_{j\pm j}$. More importantly, you should verify that for integer j, you can consistently go up and down the ladder, and thus obtain all the spherical harmonics for given value of j. However, for $j = \frac{1}{2}$:

$$J_+ Y_{\frac{1}{2}-\frac{1}{2}} \sim e^{i\phi}(\frac{\partial}{\partial\theta} \pm \cot\theta \frac{\partial}{\partial\phi})\sqrt{\sin\theta} e^{-i\phi/2} \sim \frac{\cos\theta}{\sqrt{\sin\theta}} e^{i\phi/2} \neq Y_{\frac{1}{2}\frac{1}{2}}$$

The same contradiction occurs for any half-integer j. Therefore, states with half-integer j cannot be due to the orbital angular momentum. Another way to see this is from the approach terminating the Legendre polynomial, (again analogous to a similiar approach to the Harmonic Oscillator), which was seen to yield states with integer j only–see Text).
Miraculously enough, states with half-integer angular momentum do exist (protons, neutrons, electrons, quarks,...), and what they are due to is a good question. It is easy to see, but not so easy to comprehend. that the $j = 0$ states cannot be the only fundamental building blocks, but the $j = \frac{1}{2}$ states might be.

7.1.8 Spin, and Matrix representation

We have seen that only the integer angular momentum states can be represented by state functions of coordinates, which are then acted on by differential operators. However, *all* angular momentum states can be represented by bracketing the state with the eigenstates of the angular momentum. A state $|\psi\rangle$ of angular momentum j is then represented by a (2j + 1)-dimensional vector

$$\psi_n = \langle jn|\psi\rangle$$

and operators are represented by $(2j+1) \times (2j+1)$ matrices

$$A_{mn} = \langle jm|A|jn\rangle$$

The matrix elements of $\hat{J}^2$ and $\hat{J}_z$ are trivial, the matix elements of $J_\pm^\dagger J_\pm$ provide the correct normalization, and matrix elements of $J_\pm$ serve to determine the matrix elements of J_x and J_y. We will define spin as angular momentum of a particle in its own rest frame. Particles with integer spin are called bosons, particles with half-integer spin are called fermions. Spin angular momentum of a fermion cannot be completely 'due' to the orbital angular momentum of its components.
A particle with spin can of course move in space. It will then be described by a vector (spinor) with elements $\psi(\vec{r}, t)$ which will obey the time-dependent Schroedinger equation

$$i\hbar \frac{\partial |\psi\rangle}{\partial t} = \hat{H} |\psi\rangle$$

where the Hamiltonian operator will be a $(2j+1) \times (2j+1)$ matrix.

7.1.9 Example: Behavior of Spin $\frac{1}{2}$

This example is mathematically the easiest case. To compensate for this, the physics interpretation is more difficult, as it demonstrates the fundamentally non-classical nature of half-integer spin.

First we need to establish the correct normalization of the spin states. By a procedure along the normalization of the states of SHO we obtain

$$S_{\pm}|s,m>=\hbar\sqrt{s(s+1)-m(m\pm 1)}|s,m\pm 1>$$

Then we use this to get the matrix elements of the operators S_x, S_y, S_z and S^2 - see Griffiths p. 174
Then we use the general procedure for solving a matrix eigen-equation for an N by N operator B:

$$B|\phi>=b|\phi>$$

This is equivalent to a system of N homogeneous equation for the N unknown coefficients d_m

$$\sum_m d_m(b_{mn}-b\delta_{mn})=0 \qquad n=1,N$$

This system of equations has a non-trivial solution if

$$det|b_{mn}-b\delta_{mn}|=0$$

This is a polynomial equation for b of order N, with N solutions. Corresponding to each solution there is a set of coefficients d_i corresponding to an eigenfunction $|\phi_i>$ of B.

For $s=\frac{1}{2}$ the procedure is mercifully simple, and results (as expected) into eigenvalues of

$$m_z=\pm\frac{1}{2}, m_x=\pm\frac{1}{2}, m_y=\pm\frac{1}{2}$$

corresponding to eigenvectors

$$[(0,1),(1,0)],[\frac{1}{\sqrt{2}}(1,\pm 1)],[\frac{1}{\sqrt{2}}(1,\pm i)]$$

Note the three different ways in which orthogonality is achieved.
Next obtain the expression for the eigenfunction $|m_x=+\frac{1}{2}\rangle$ in the coordinate frame rotated around the z-axis by ϕ:

$$|\psi'\rangle=\frac{e^{i\phi/2}}{\sqrt{2}}(1,e^{-i\phi})$$

and use it to answer the following questions:
a) Determine $\langle S_{x'}\rangle, \langle S_{y'}\rangle$ and the vectors (a',b') (in the same manner as explained above for spin-1) for angles ϕ from 0^0 to 720^0 in steps of 90^0. This (especially the situation at 360^0) probably makes somewhat less immediate sense than the spin-1 case (but that is OK– remember this is Quantum Mechanics!)

b) Optional: Contrast all this with the case of an electron originally at rest with $m_x = \frac{1}{2}$ in magnetic field $(0, 0, B)$, which is described by the time-dependent Schroedinger equation with Hamiltonian $H = -\vec{M} \cdot \vec{B}$, where $\vec{M} = -g(e\hbar/2mc)\vec{\sigma}/2$, resulting in

$$|\psi(t)\rangle = \frac{e^{-i\omega t/2}}{\sqrt{2}}(1, e^{-i\omega t})$$

Note that you are (or rather, the magnetic field is) doing an 'active rotation' (rotating the object). Note also that a concept of 'torque' would appear in the classical limit, much as the concept of 'force' emerged in a classical limit of an electron deflected by the electric field.
c) A Spin $\frac{1}{2}$ particle is prepared with spin-up in a given direction, and you measure the spin projection along a direction making an angle θ with respect to the original direction. What is the probability that you find spin-up? (We will need this when discussing the EPRB puzzle).