Lectures on Physics Chapter II: Probability Amplitudes

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Abstract

The special problem we try to get at with these lectures is to maintain the interest of the very enthusiastic and rather smart people trying to understand physics. They have heard a lot about how interesting and exciting physics is—the theory of relativity, quantum mechanics, and other modern ideas—and spend many years studying textbooks or following online courses. Many are discouraged because there are really very few grand, new, modern ideas presented to them. Also, when they ask too many questions in the course, they are usually told to just shut up and calculate. Hence, we were wondering whether or not we can make a course which would save them by maintaining their enthusiasm. This paper is a draft of the second chapter of such course.

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Preface¹

To explain what a probability amplitude might actually be, one has to get into the specifics of the situation: explaining how an ammonia maser might work as opposed to, say, having a look at Schrödinger's hydrogen atom, are very different endeavors. However, despite the very different physicality of these two systems, they allow for a similar approach in terms of their *quantum-mechanical analysis*. The question is: why is that so? The preliminary answer is this: both phenomena involve periodicity and regularity – some *oscillation* – which, mathematically, can be represented by the same mathematical functions: a sinusoid or – what Nature seems to prefer – a combination of a sine and a cosine: Euler's $a \cdot e^{i\theta} = a \cdot (\cos\theta + i \cdot \sin\theta)$ function.²

In our previous lecture (chapter I), we showed how we may use the elementary wavefunction to represent an elementary particle: we looked at the electron and its smaller more massive and unstable variant—the muon. We also discussed protons and neutrons—modeling the latter as composite particles, which are stable inside of a nucleus only.³ We concluded all should be thought of as ring currents which can, effectively, be represented by Euler's function: we may, effectively, interpret $\mathbf{r} = a \cdot e^{i\theta}$ as the $\mathbf{r} = (\mathbf{x}, \mathbf{y})$ position of the electric charge as it orbits around some center with radius $a = \hbar/mc$ and frequency $\omega = E/\hbar$. There is more than one way to represent this model but we think the easy formulas and derivation below do the trick rather well⁴:

$$\begin{cases} c = a\omega \\ E = \hbar\omega \end{cases} \Rightarrow \frac{c}{a} = \frac{E}{\hbar} \iff a = \frac{\hbar c}{E} = \frac{\hbar}{mc}$$

This should – by now – come across as rather intuitive: Einstein and de Broglie's intuition in regard to the wave-nature of matter was essentially correct, but they should have thought of a stationary circular

¹ This is the second chapter of a rather ironic re-write of <u>Feynman's iconic lectures series on quantum mechanics</u>. The reader will not be able to make sense of this chapter without a thorough reading of <u>our first chapter</u>.

² The sine and cosine function are the same function but with a phase difference of 90 degrees. We, therefore, may think of some kind of perpetuum mobile: two oscillations working in tandem and transferring (potential and/or kinetic) energy to and from each other. We developed this metaphor in <u>one of very first papers</u> which, if only because of its naïve simplicity, we may still recommend.

³ The negative charge inside of a neutron may help to keep the nucleus together. We can, therefore, think of this charge as some kind of *nuclear glue*. We tentatively explored this idea in a paper: *Electrons as gluons?* The basic idea is this: the electromagnetic force keeps electrons close to the positively charged nucleus and we should, therefore, not exclude that a similar arrangement of positive and negative charges – but one involving some strong(er) force to explain the difference in scale – might exist within the nucleus. One can effectively never find a proton pair without one or more neutrons: the main isotope of *helium* (⁴He), for example, has a nucleus consisting of two protons and two neutrons, while a helium-3 (³He) nucleus consists of two protons and one neutron. When we find a pair of nucleons, like in deuterium (²H), this will always consist of a proton and a neutron. The idea of a negative charge acting as an in-between to keep two positive charges together is, therefore, quite logical. Think of it as the opposite of a positively charged nucleus keeping electrons together in a multi-electron atom.

⁴ This derivation shows our model applies Wheeler's 'mass without mass' idea: all of the mass is in the energy of the oscillation. A dimensional analysis of the two sides of the $c/a = E/\hbar$ equation is interesting too. We have the inverse of a time unit on the left-hand side because we are dividing a (tangential) velocity by a distance unit (the Compton radius): $c/a = \omega = 2\pi/f = 2\pi/T$. The latter is, effectively, the inverse of what is sometimes referred to as an <u>angular period</u> (T/2 π), as opposed to a <u>linear period</u> (T). Energy is expressed in N·m, while Planck's (reduced) quantum of action is expressed in N·m·s. Hence, these physical dimensions make sense.

oscillation instead of trying to adapt the *linear* wave concepts that we associate with photons or, more generally, with electromagnetic and all other physical waves. The conceptual *switch* that has to be made here is to think of *c* as a tangential rather than a linear velocity: that is all—nothing more, nothing less. So let us turn the page on this and move to the next—the topic of this chapter: the concept of probability amplitudes.

Indeed, using Euler's function to describe a particle and using it in what is commonly referred to as a probability amplitude are two *very* different things. Let us look at the latter in more detail by analyzing a particular two-state system and then see whether or not we can generalize whatever results we might get.

2-1 A two-position system

A state may refer to a position so we will take an easy two-position system⁵ as an example of a two-state system: an ammonia molecule in an electric field (**Figure 1**).⁶

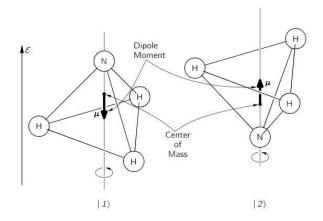


Figure 1: An ammonia molecule in an electrostatic field⁷

We choose this example for the same reason as why Feynman uses it in his introduction to two-state systems: the ammonia maser is one of the very first practical applications of the theory of quantum mechanics. It was built in the early 1950s and its inventor, Charles Townes, wanted the m in m aser to refer to m of m mechanism is similar to that of a laser: the m in m maser effectively refer to the same as in m mechanism is similar to that of a laser: the m in m maser effectively refer to the same as in m mechanism is similar to that of a laser: the m in m maser effectively refer to the same as in m mechanism is similar to that of a laser: the m in m meser effectively refer to the same as in m meser (m mechanism is similar to that of a laser: the m in m meser effectively refer to the same as in m meser (m mechanism is similar to that of a laser: the m in m meser effectively refer to the same as in m meser (m meser effectively refer to the same as in m meser (m meser effectively refer to that m meser effectively refer to the same as in m meser effectively refer to that m meser effectively refer to the same as in m meser effectively refer to that m meser effectively refer to the same as in m meser effectively refer to the same as in m meser effectively refer to that m meser effectively refer to the same as in m meser effectively refer to that m meser effectively refer to the same as in m meser effectively refer to the m meser effectively refer to the m meser effectively refer to m meser effectively refer to

⁵ In case the reader wonders: yes, we just invented this term.

⁶ In case you wonder what an electric field actually is, we mean an *electrostatic* field, which originates from static charges—as opposed to a magnetic field, which originates from *moving* charges.

⁷ We gratefully acknowledge the online edition of Feynman's Lectures for this illustration.

The state concept

Figure 1 clearly shows *position* states $|1\rangle$ and $|2\rangle$ have nothing to do with the spin state of the molecule as a whole: that is the same in the right- and left-hand side illustrations, as shown by the rotation arrow around the symmetry axis of this molecule. There is *no spin flip*, and you should also *not* think that this NH₃ molecule goes from state $|1\rangle$ to $|2\rangle$, or vice versa, by flipping over *as a whole*—by changing its orientation its space, that is. No! What happens here is that the nitrogen atom (N), *somehow*, manages to tunnel through the plane that is formed by the three hydrogen atoms (H₃). We will come back to this. Before we do so, we should note that we have not introduced much quantum-mechanical symbolism yet, so let us quickly do this now.

The $|1\rangle$ and $|2\rangle$ notation represent *physical* base states here. This $|\phi\rangle$ notation is known as the *ket* in Dirac's *bra-ket* notation and always refers to some *initial* state that may or may not change. In contrast, the $\langle \chi |$ notation is a *bra*-state and refers to some *final* state. These initial and final states are separated by time – states may change as the clock keeps ticking without us intervening in any way – or, alternatively, because we put the particle through some apparatus, process, or force field—which we may denote by A or S. We may, therefore, say some apparatus or process will *operate* on some (initial) state $|\phi\rangle$ to *produce* some (end) state $\langle \chi |$. We write that like this:

$$\langle \chi | A | \phi \rangle$$

Note you need to read this from right to left, like Arabic or Hebrew. Because this looks quite formidable, we should give a practical example: if the electric field – the $\mathcal E$ in the illustration⁸ – is very strong or, if it is being applied long enough, then an atom in the $|1\rangle$ state will go into the $|2\rangle$ state so as to ensure the electric dipole moment of the ammonia molecule (μ) is aligned with the electric field.⁹ This is all quite logical because the energy of the ammonia molecule as a whole will be lower if and when it can align its dipole moment with the field.

We should, of course, note that the notion of an energy difference between the two states can only be defined with reference to some external field: we can say that the NH_3 molecule has more energy in state $|1\rangle$ than in state $|2\rangle$ because its polarity in state $|1\rangle$ opposes the field. We may, therefore, say that the external field establishes the frame of reference: what is up or down, left or right, and back or front can, effectively, only be defined with a reference to this externally applied field. This may seem to be a trivial philosophical remark but physicists sometimes seem to lose sight of this when doing more

⁸ We usually use E for an electric field but we use the E symbol here so as to ensure there is no confusion with the E that is used to denote energy.

 $^{^9}$ Notation is tricky once again because we use the same μ symbol to refer to a *magnetic* moment in another context. However, we trust the reader is smart enough to know what is what here.

¹⁰ The reader may think this electric field has the same axis of symmetry as the NH₃ molecule and that we may, therefore, not be able to distinguish left from right or vice versa. However, this problem is solved because it is assumed we have knowledge of the spin direction (see the rotation arrow in **Figure 1**). We also know what is back and front because we are doing this experiment and we, therefore, have some idea of our own relative position vis-à-vis the electric field and the ammonia molecule. In short, we may say that the experiment as a whole comes with the relevant frame of reference for the measurement of position, energy and whatever other physical property or quantity we would want to observe here.

complicated abstract mathematical calculations.

We need to make a second remark here: are we talking the dipole moment of the molecule or the nitrogen atom? It is an *electric* dipole moment, so it must be the dipole moment of the molecule, right? Atoms may have a magnetic moment¹¹ but they would *not* have an electric moment, right? The answer is: yes, and no. Something must cause the ammonia molecule to be *polar* and that something is the configuration of the system: nitrogen has 7 electrons, which are shared with the hydrogen nuclei in covalent bonds. A covalent bond blurs the idea of an electron belonging to one atom only. You may think of it like this: the *valence* electrons allow the hydrogen to also (partly) fill its shell with paired electrons.

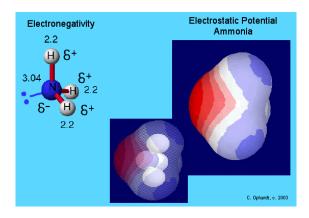


Figure 2: The charge distribution in an ammonia molecule¹²

We will let you *google* more details of the structure of this *system*.¹³ At this point, you should just note an analysis in terms of individual atoms is not all that useful: the ideas of positively charged nuclei and electron densities are far more relevant than the idea of an individual nitrogen atom flipping through some potential barrier—although the latter idea is what we are going to be talking about, of course! Just remember this when you are getting confused or if we would happen to be using non-specific language ourselves¹⁴: we are talking the state of the ammonia *molecule* (or the molecular *system*, we should say) but this state – in this discussion, at least – is determined by the relative position of the nitrogen.

¹¹ All atoms with an uneven number of electrons have a magnetic moment because electrons in a *pair* (remember the standard configuration of a electron orbital has *two* electrons) will have opposite spin. The silver atoms which Otto Stern and Walther Gerlach sent through their apparatus in 1922, for example, have 47 electrons. It is interesting to note that a similar line-up happens if we consider the nucleus alone: when applying an external magnetic field, *pairs* of nucleons will line up so as to lower the joint energy of the system.

¹² We gratefully acknowledge the source of this illustration: the <u>virtual Elmhurst College Chemistry Book</u>, Charles H. Ophardt, 2003.

¹³ There are various ways to look at it. The <u>Chembook</u> illustration shows a lonely electron pair but you should note the nitrogen atom also wants fully-filled (sub-)shells. Its 1s and 2s subshells have two, but the *three* 2p (subshells) each lack one electron, and then the 1s orbitals of the *three* hydrogen atoms lack one too. We, therefore, have five valence electrons. The nitty-gritty of the charge distribution is, therefore, quite complicated.

¹⁴ This inevitably happens when getting into quantum-mechanical descriptions so we will not apologize for it.

Potential wells and tunneling

If there is an energy difference between state $|1\rangle$ than in state $|2\rangle$, then how can we explain the nitrogen atom tends to stay where it is? How is that possible? The reader will be familiar with the concept of a potential well – if not, *google* it – and the reader should, therefore, note that the potential energy of the N atom will effectively be higher in state $|1\rangle$ than in state $|2\rangle$ but, because of the energy barrier (the *wall* of the potential well), it will tend to stay where it is—as opposed to lowering its energy by shifting to the other position, which is a potential well itself!

Of course, you need to read all of the above carefully: we wrote that the nitrogen atom will *tend* to stay where it is. From time to time, it does tunnel through. The question now becomes: when and how does it do that? That is a bit of a mystery, but you should think of it in terms of *dynamics*. We modeled particles as *charges in motion*. Hence, we think of an atom as a dynamic system consisting of a bunch of elementary (electric) charges. These atoms, therefore, generate an equally dynamic electromagnetic field structure. We, therefore, have some *lattice* structure that does not arise from the mere *presence* of charges inside but also from their pattern of *motion*. ¹⁵

Can we model this? Feynman did not think this was possible.¹⁶ In contrast, we believe recent work on this is rather promising—but we must admit it has not been done yet: it is, effectively, a rather complicated matter and, as mentioned, work on this has actually just started!¹⁷ We will, therefore, not dwell on it here: you should do your *PhD* on it! The point is this: you should take a dynamic view of the fields surrounding charged particles. Potential barriers – and their corollary: potential *wells* – should, therefore, not be thought of as static fields: they vary in time. They result from or more charges that are moving around and thereby create some *joint* or superposed field *which varies in time*. Hence, a particle breaking through a 'potential wall' or coming out of a potential 'well' is just using some temporary opening corresponding to a very classical trajectory in space and in time.¹⁸

There is, therefore, no need to invoke some metaphysical Uncertainty Principle: we may not know the *detail* of what is going on—but we should be able to *model* it using classical mechanics!

Modeling uncertainty

The reader should, once again, note that the *spin* state or *angular momentum* state is the same in the $|1\rangle$ and $|2\rangle$ states. Hence, the only *uncertainty* we have here is in regard to the position of the nitrogen atom (N) vis-à-vis the plane that is formed by the three hydrogen atoms (H). As long as we do not actually investigate, we cannot know in what state this nitrogen atom – or the molecule as a whole –

¹⁵ You should also do some thinking on the concept of charge *densities* here: the different charge densities inside of the ammonia molecule do *not* result from static charge distribution but because the negative charges inside (pointlike or not) spend more time here than there, or vice versa.

¹⁶ We will soon quote his remarks on this, *verbatim*, so be patient for the time being!

¹⁷ In case you would want to have an idea of the kind of mathematical techniques that are needed for this, we hereby refer you to <u>a recent book on what is referred to as nuclear lattice effective field theory (NLEFT)</u>.

¹⁸ You should also do some thinking on the concept of charge *densities* here: the different charge densities inside of the ammonia molecule do *not* result from static charge distribution but because the negative charges inside (pointlike or not) spend more time here than there, or vice versa.

actually is. Paraphrasing Wittgenstein¹⁹, we can say our theory can only tell us what *might be* the case: it is only some measurement that can establish what actually *is* the case. We can, of course, also *prepare* the NH₃ molecule by *polarizing* it in a strong-enough electric field. However, in either case, we will, of course, *disturb* the system and, by doing so, put it in some new state.

We do not want to do that. Instead, we will try to model **our** uncertainty in regard to the position of the nitrogen atom, *in the absence of a measurement or polarization*, by thinking of it in very much the same way as the proverbial cat in the equally proverbial Schrödinger box: because we do not *know* if it is dead or alive, we can only associate some abstract *logical* state with it—a combination of being dead and alive *which exists in our mind only*. Fortunately, the state of the ammonia molecule is much less dramatic or critical as that of Schrödinger's cat, and we will simply write it as:

$$|\phi\rangle = C_1 \cdot |1\rangle + C_2 \cdot |2\rangle$$

This looks like a very simple formula but it is actually quite frightening what we are doing here:

1. The $|1\rangle$ and the $|2\rangle$ states are (logical) representations of what we think of as a *physical* state: they are *possible realities*—or *real possibilities*, whatever term you would want to invent for it. When using them in a mathematical equation like this, we will think of them as state *vectors*. There is a lot of mathematical magic here, and so you should wonder: what *kind* of vectors are we talking about? Mathematicians refer to them as *Hilbert* vectors²⁰ and **Figure 3** shows why Schrödinger liked them so much: whatever they might represent, we can effectively add and multiply them, *somehow*.

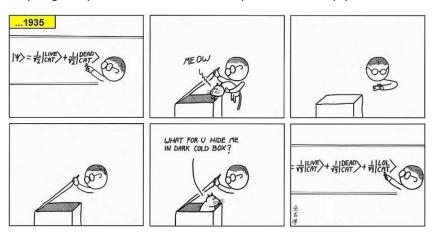


Figure 3: Adding cats dead, alive or in-between²¹

¹⁹ We refer to Wittgenstein's theses in his *Tractatus Logico-Philosophicus*, which our reader may or – more likely – may *not* be familiar with.

²⁰ This is actually incorrect: they are referred to as being vectors in a Hilbert *space*. It depends on what you think of as being special: we think it is the vectors, rather than the space, so we add Hilbert's name to the vectors rather than the space. In case you wonder, David Hilbert is *not* English. He was German. He died in 1943 and his tomb carries these words: *Wir müssen wissen. Wir werden wissen*, which we may translate as: "*We must know. We will know.*"

²¹ We saw <u>this cartoon on *MathExchange*</u>, which references <u>AbstruseGoose</u> as the source. The date on this cartoon (1935) is somewhat weird: Paul A.M. Dirac published the first edition of his *Principles of Quantum Mechanics* in 1930. It may also be mentioned that, while the cat seems to be Schrödinger's alright (the man who puts the cat in

It is really like adding apples and oranges. What do you get when you do that? Some fruits, right? © So we will talk about fruits but we should not forget they consist of apples and oranges. That is the fruit menu of today. You might get grapes and bananas tomorrow.

2. Where were we? Yes. Physical states. In this case, we multiply them with C_1 and C_2 , which are usually referred to as complex numbers (or complex functions, to be precise) but – because we are multiplying them with these state vectors – you will want to think of them as vectors too. That is not so difficult: complex numbers have a direction and a magnitude, so they are vectors alright!

So what happens when we multiply apples or oranges with some number? We get two apples, or half an orange. It depends on the fruit and the number. But so here we multiply with some *complex* number. That is hard to visualize: we know a complex number includes the idea of an orientation in space (a complex number is defined by its length *and* its direction in space) but this idea does not help us very much here.

3. The sum of the $C_1 \cdot |1\rangle + C_2 \cdot |2\rangle$ then gives us the $|\phi\rangle$ state. This is a *logical* state: it exists in our mind only.²² Why in our mind only? Because we are not trying to measure anything so we are in a state of uncertainty ourselves: we think of some fruit but we are not being specific—we are not talking apples or oranges here.²³

Let us stop the philosophy here: let us present a few calculations instead.

the box wears Schrödinger's glasses), the bra-ket notation was invented by Dirac. Schrödinger's seminal paper for the 1927 Solvay Conference (*La Mécanique des Ondes*) makes use of wave *functions* only. One of the reasons we like Feynman's *Lectures on Quantum Mechanics* is him going from discrete states (mostly two-state systems) to then generalize to an infinite number of discrete states what, in practice, amounts to continuous states, which are modeled by wave mechanics—as opposed to matrix mechanics. It, therefore, bridges the two approaches, which complement each other, of course!

²² You may think we should distinguish a third physical state: the state of our nitrogen atom while it is moving from position 1 to position 2 or vice versa. However, we assume this happens so quickly that the time that is spent in this state is negligible. We think the state itself is, therefore, negligible.

²³ We are not talking an apple-orange smoothie either!

2-2 An intuitive explanation

What is that we want to calculate?

Because calculation is very boring and, more importantly, because it is important to not lose track of whatever is that we want to calculate²⁴, we will give you a *sneak* preview of the result that we want. It looks like this—two probabilities 'sloshing back and forth', as Feynman would say, as a function of time:

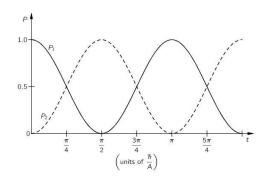


Figure 4: Probabilities sloshing back and forth²⁵

The illustration triggers an obvious question: how do we know our nitrogen atom will be at position 1 or, we should say, in state $|1\rangle$ at t=0, π , 2π ,... as measured in the relevant unit here, which is \hbar/A ? The graph assumes we do: perhaps we had switched on some strong electric field for a while so as to polarize the ammonia molecule—and then we switched it off at t = 0. It does not matter—not at this point, at least: probabilities are probabilities, so there is, perhaps, no reason why we must be so sure. The important thing is the *periodicity* of these functions: the cycle time $\pi\hbar/A$.²⁶ That is what we want to calculate.

So how do we find that cycle time, and what is the value of A?²⁷

We will tell you. Let us just quickly also answer the latter question: A is equal to $\mu \mathcal{E}_0$. Of course, this is no real answer because the question now becomes: what is \mathcal{E}_0 ? We can, effectively, *measure* the (electric) dipole moment μ , but \mathcal{E}_0 must be related to the strength of the external field \mathcal{E} . What field are or should we be applying here? Feynman is rather vague about that, but we get some kind of answer in the next lecture²⁸: it turns out that, when actually operating an ammonia maser, we will apply an electric field

²⁴ You will be surprised but people do sometimes forget what they want to get at. *I* sometimes do, at least. 😊

²⁵ We gratefully acknowledge the online edition of Feynman's Lectures for this illustration too.

²⁶ When expressing the cycle time, the factor 2 vanishes because we must measure the cycle time from peak to peak, or from trough to trough.

²⁷ We will quickly tell you the answer: A is equal to $\mu \mathcal{E}_0$. Of course, this is no real answer because the question now becomes: what is \mathcal{E}_0 ? We can, effectively, measure the (electric) dipole moment μ , but \mathcal{E}_0 must be related to the strength of the external field \mathcal{E} . What field? Feynman is remarkably and mysteriously vague about that. $\pi\hbar/A$

²⁸ This chapter deals with a number of chapters in Feynman's Lectures (about half of his lectures discuss some kind of two-state system) but Feynman's Chapter 8 and 9 are the basic ones, because they both deal with the mechanics of the ammonia maser—which we, just like Feynman, think of representing the basics of a quantummechanical discussion of any two-state system.

that varies sinusoidally with a frequency that is equal or very near to the so-called resonant frequency of the molecular transition between the two states. So this is what Feynman gives us²⁹:

$$\mathcal{E} = \mathcal{E}_0 \cdot 2\cos(\omega t) = \mathcal{E}_0 \cdot (e^{i \cdot \omega t} + e^{-i \cdot \omega t})$$
 and $\omega = \omega_0 = 2A/\hbar$

The question now becomes: what *is* that resonant frequency? Feynman just writes it down—with no explanation: . That's what was experimentally measured apparently.

The reader will (or should) note there is some circularity in the argument here, but we cannot help that: we stick quite closely to Feynman's rather *heuristic* approach to explaining quantum math, and so it is what it is and we request the reader to try to get through it and make sense of it.

What are those amplitudes?

Let us, before we move to the meat of the matter, also give you a sneak preview of the result we should obtain for those C_1 and C_2 coefficients: these weird probability *amplitudes*. We are going to get this:

$$C_1 = e^{-i\frac{E_0}{\hbar}t}\cos\left(\frac{A}{\hbar}t\right)$$

$$C_2 = i \cdot e^{-i\frac{E_0}{\hbar}t} \sin\left(\frac{A}{\hbar}t\right)$$

Time is the variable, so you may want to think of the $e^{-i\frac{E_0}{\hbar}t}$ function as representing the hand of an old-fashioned stopwatch: its length is 1 (unity) and its angular or rotational frequency is equal to E_0/\hbar . What is E_0 ? Feynman defines E_0 as the average energy of the ammonia molecule but you should just think of it as an average tout court: the average of E_0 + A and E_0 – A:

$$\frac{E_0 + A + E_0 - A}{2} = E_0$$

Why are we saying this? Because we do not have to be specific about *what* energy we are talking about when introducing E₀: we may or may not include the *rest* mass of the nuclei, for example³⁰. The point is: what we include or not, does not matter: our choice will determine the *zero* point on the energy scale but there is no need in our calculations for an *absolute* zero point: all that matters is this energy *difference* A.³¹ Let us get back to those amplitudes.

$$e^{i\cdot\theta} + e^{-i\cdot\theta} = \cos\theta + i\cdot\sin\theta + \cos\theta - i\cdot\sin\theta = 2\cdot\cos\theta$$

$$e^{i\cdot\theta} - e^{-i\cdot\theta} = \cos\theta + i\cdot\sin\theta - \cos\theta + i\cdot\sin\theta = 2\cdot i\cdot\cos\theta$$

²⁹ The reader should note the interesting formula for the sum and/or the difference of *conjugate* complex numbers or functions here, because we may need it later:

³⁰ We may think of the nuclei as the *stationary* components of the molecule, so it makes sense to only talk about their rest mass. In contrast, we think of the electrons as pointlike charges whizzing around at lightspeed, so all of their energy is kinetic. We also have energy in the electromagnetic field(s), of course! Any other energy? Yes: vibrational, rotational, whatever! Why are we making things complicated? We are not. We just want to point out that the energy concept can be quite complicated when discussing a full-blown *system* of particles!

³¹ You may think we should get into trouble when setting E_0 to zero, because the argument in this complex exponential vanishes: $e^0 = 1$. Our stopwatch stops! We will let you think about this as an exercise: you should walk

The $\cos(A \cdot t/\hbar)$ function is going to *modulate* the length of our stopwatch hand: it goes from 1 (for t = 0) to zero (for $t = \pi/2$), to -1 ($t = \pi$), zero again ($t = 3\pi/2$), and back to 1 ($t = 2\pi$). How can a length be negative? It cannot be, of course: the minus sign is directional only: -1 is +1 in the opposite direction.³²

Let us now look at the function for C_2 : the $i \cdot e^{-i\frac{E_0}{\hbar}t}$ function is the same stopwatch hand but it is 90 degrees out of phase with the other stopwatch. We have the same phase difference between the sine and cosine functions that we are multiplying these stopwatch hands with.³³

We must note a last thing: the periodicity of the probability functions (P_1 and P_2) is π , so that is *half* of the usual period of (co)sine and complex exponentials (2π). In other words, it is *half* of the period of our C_1 and C_2 amplitude functions. That is why the factor 2 in the $\omega = \omega_0 = 2A/\hbar$ formula for the resonant frequency makes sense: the resonant frequency and the *probability* functions have the *same* period (π). Of course, a *squared* sine (or cosine) also has the same period (π). The math is wondrous but works!

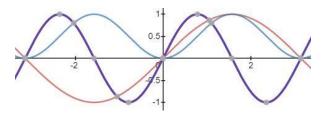


Figure 5: The $sin(\theta)$, $sin(2\theta)$ and $sin^2(\theta)$ functions and their periodicity³⁴

Before we present the quantum-mechanical *machinery* – Hamiltonian matrix and all that – we should make one more point. It is a very simple one. We obviously have some kind of oscillator here: a positively charged nucleus flipping back and forth and dragging some negative charge with it as it does its dance. We may, therefore, wonder we could, perhaps, just use the Planck-Einstein relation once more to model all of this. If everything inside of this molecule – the electrons, protons, neutrons, and the fields in-between them – have some frequency which is given by the Planck-Einstein relation ($\omega = E/\hbar$) – because we are talking *stable* stuff, right?³⁵ – then we might just try to use the Planck-Einstein relation once again to determine the frequency of *this* particular system, isn't it?

through the math of this chapter once more when you are done with it and check what an $E_0 = 0$ assumption would do to it. You should find it does not matter—but it might take a while before you see why.

 $^{^{32}}$ This may come across as a trivial remark but the point is quite deep, because we should also note we can go from +1 to -1 in clockwise or in counterclockwise direction: these are two opposite rotations – modeling very different things, in other words. Unfortunately, mainstream quantum theorists usually treat them as common phase shifts. See our paper on <u>Euler's Wavefunction and the Double Life of -1</u>, which also deals with the *false* 720-degree symmetries mainstream quantum theorists play with.

³³ This sounds trivial too but we request the reader to quickly verify the relations: $\sin(\theta) = \cos(\theta - \pi/2)$ and $i \cdot e^{-i \cdot \theta} = i \cdot e^{-i \cdot \theta} = e^{i \cdot \pi/2} \cdot e^{-i \cdot \theta} = e^{-i \cdot (\theta - \pi/2)}$ so as to get a feel for the *geometry* of these coefficients and wavefunctions.

³⁴ We gratefully acknowledge the online <u>Desmos.com graphing tool</u>.

³⁵ See the first chapter of this two-chapter series: stable particles are stable because their frequency is right on—their energy is in the oscillation, so they *must* be right on, of course! In contrast, unstable systems die out, so to speak, or, else, fragment into stable(r) sub-systems: transients, which then further disintegrate into stable

The thought is very logical – so we think – entirely justified: the energy difference here resembles the energy difference between, say, two electron orbitals in the Rutherford-Bohr model of an atom and we may, therefore, calculate the frequency as:

$$\omega = \frac{\Delta E}{\hbar} = \frac{2A}{\hbar}$$

Why the factor 2, and what is the relation with \mathcal{E}_0 ? We are *not* calculating an average here, so there is no 1/2 factor: $E_0 + A - (E_0 - A) = 2A$, and the difference between $+\mathcal{E}_0$ and $-\mathcal{E}_0$ is $2\mathcal{E}_0$ as well, isn't it? Yes. And no. The 2A makes sense, but the $2\mathcal{E}_0$? Perhaps we should think of it like this: if A is the potential barrier, then we need a field that is *at least* as strong to break through it, right? Maybe. Maybe not. Let us be precise here. The argument should, perhaps, more be like this: the energy of an electric dipole moment μ^{36} in some electric field $\boldsymbol{\mathcal{E}}$ is equal to $\mu \cdot \boldsymbol{\mathcal{E}} \cdot \cos \alpha$ and, hence, to *flip* the dipole moment, we will need an energy that is equal to (at least) $2\mu \mathcal{E}^{.37}$ So we have a factor 2 here too... But - Hey! - what is this potential barrier, exactly? The dipole moment and this potential barrier must be two sides of the same coin, isn't it?

Good thinking! We can now, effectively, not worry too much about Feynman casually mentioning A should be equal to $\mu \mathcal{E}_0$. In fact, we should probably *define* \mathcal{E}_0 as $\mathcal{E}_0 = A/\mu$.

Does stuff like this matter? A and μ are the *physical* variables that characterize the system: the \mathcal{E}_0 field is just some field that we – the observer – applies to it. The argument should, therefore, be driven by A and μ , not by \mathcal{E}_0 .³⁸

The Planck-Einstein explanation

What we just wrote above amounts to an intuitive classical explanation of the maser: the Planck-Einstein relation gives us the resonant frequency of the maser $-\omega_0 = \Delta E/\hbar = 2A/\hbar = 2\mu \mathcal{E}_0/\hbar$ — and now we need to get those probabilities. What are probabilities anyway? A probability is some number between 0 and 1 and, in this case, we have $two - P_1$ and P_2 — and we need them to slosh back between each other. We can now easily calculate the *period* of the probability (T) from the $\omega = 2\pi \cdot f = 2\pi/T$ flipping frequency:

$$\omega_0 = 2\pi \cdot f = \frac{2\pi}{T} = \frac{2A}{\hbar} \iff T = \frac{\hbar}{A}\pi$$

So that is what **Figure 4** shows: when expressing time in units equal to \hbar/A , the periodicity of these probability functions is equal to π . Why a *squared* sine and cosine? That is just geometry: probability

elementary particles. Whatever excess energy there may be – electromagnetic or strong – radiates away as photons or neutrinos.

³⁶ The dipole moment is a *vector* quantity: it has got direction and, hence, we write it in **boldface**. The same is true for the electric field.

³⁷ The α is the angle between the dipole and field directions. Hence, the energy will be equal to $-\mu\mathcal{E}$ when the dipole is *aligned* with the field direction (*lowest* energy possible) and $\mu\mathcal{E}$ when its direction is opposite to that of the field (it can then lower it by flipping over). The energy difference is, therefore, $2\mu\mathcal{E}$.

³⁸ Why do we mention this? Because Feynman does *not* do that, and we want to alert the smart student to <u>the</u> <u>difference between a theory, a calculation and an explanation</u>.

functions should be smooth but cannot be negative and, yes, the periodicity of the sine and cosine is 2π . So what is the point?

The point is this: these probability amplitudes are, perhaps, just irrelevant. We can calculate them from the probabilities by taking their *square root*, of course, but why would we do that? No one knows what these amplitudes actually represent anyway, right?

Right.

[...]

So what? Do we need all of that quantum-mechanical machinery? Frankly, we do not think so, but we are here to give it to you and so that is what we will do. Let us get on with it.

2-3 Amplitude math

Coefficients and the Hamiltonian matrix

If someone has talked to you about quantum mechanics at all, chances are he or she mentioned the Hamiltonian. So what is this (in)famous Hamiltonian? It has got little or nothing to do with *classical* Hamiltonian mechanics, so we recommend you do *not* try to compare too much: one can, actually, but it will probably only confuse you if you try to do this at this stage of your studies.³⁹ To explain what it is all about, we will review that formula we started out with:

$$|\phi\rangle = C_1 \cdot |1\rangle + C_2 \cdot |2\rangle$$

You may want to think of $C_1 \cdot |1\rangle$ and $C_2 \cdot |2\rangle$ as two vector *products*, and you may think this is consistent with the notion of probabilities being calculated as the (absolute) square of some probability amplitude. To be precise, a probability will generally be calculated as something like this⁴⁰:

$$P = |\psi|^2 = |a \cdot e^{i\theta}|^2 = |a|^2 \cdot |e^{i\theta}|^2 = a^2$$

$$\left|e^{i\theta}\right| = +\sqrt{\cos^2\theta + \sin^2\theta} \Leftrightarrow \left|e^{i\theta}\right|^2 = \left|+\sqrt{\cos^2\theta + \sin^2\theta}\right|^2 = \left|+\sqrt{1}\right|^2 = 1$$

³⁹ Sir William Rowan Hamilton, whose name is associated with this, died long ago (in 1865, or be precise) and was, therefore, aware of *classical* mechanics only. In fact, *Hamiltonian mechanics* refers to a reformulation of good old Newtonian mechanics. Most relevant for quantum mechanics is his great work in regard to complex number theory: he actually extended the concept of complex numbers to <u>quaternions</u>, which have found renewed usage in the programming of computer video games.

⁴⁰ You should probably review some of the basic rules in regard to complex numbers, basic trigonometry, and various other related and unrelated rules, such as the rule for squaring absolute values and all that. Note that we must not necessarily assume the coefficient a is a real but *positive* number—although it usually is: $|a|^2$ will *always* be equal to a^2 , even if a is a *negative* real number. As for $|e^{i\theta}|^2$ being equal to 1, we should remind ourselves of the definition of the absolute value of a complex number: it is the *length* of the associated vector, which we find by taking the *positive* square root of the sum of the squares of cosθ and sinθ. Let us write this out for clarity:

We may remind ourselves also of some other formula here, which might or might not help us to get a more intuitive grasp of the rather special math we are going to use—Pythagoras' formula in *vector* format⁴¹:

$$c^2 = a^2 + b^2 \iff c^2 = a^2 + b^2 \iff |c|^2 = |a|^2 + |b|^2 \iff |c| \cdot |c| = |a| \cdot |a| + |b| \cdot |b|^2$$

Needless to say, the a and b vectors are orthogonal or perpendicular vectors here. It is interesting to write c more generally as the sum of any two vectors a and b – orthogonal or not – and to square this sum:

$$c^2 = (a + b)^2 = a^2 + b^2 + 2a \cdot b = a^2 + b^2 + a \cdot b \cdot \cos\theta = a^2 + b^2$$
 if and only $\theta = \pm \pi/2$

We get the same result: Pythagoras formula is valid if and only if **a** and **b** are orthogonal vectors. This condition is valid in quantum math too: a system – any system, really – will always be described in terms of base states which will be orthogonal one to another. This matches the condition of *linear independence* for any set of base vectors in any mathematical space. So far, so good.

Let us think about what we wanted to think about here: those coefficients C_1 and C_2 . They will be complex functions of time as well, so we should write them as $C_1(t)$ and $C_2(t)$. We will also have time derivatives $dC_1(t)/dt$ and $dC_2(t)/dt$. What can we do with this? I must refer to Feynman's lecture on how states change with time⁴² here for a great but rather complicated abstract logical argument which involves time as an apparatus. I will just note Feynman's introduction to it—and the grand result, of course:

"We have already talked about how we can represent a situation in which we put something through an apparatus. Now one convenient, delightful "apparatus" to consider is merely a wait of a few minutes; that is, you prepare a state φ , and then before you analyze it, you just let it sit. Perhaps you let it sit in some particular electric or magnetic field—it depends on the physical circumstances in the world. At any rate, whatever the conditions are, you let the object sit from time t_1 to time t_2 ."

Then follows the mentioned brilliant exposé—which we will not copy here. 43 We just copy the grand

⁴¹ We are deliberately a bit sloppy in using the *dot* for a product, or not—because we want you to think about the difference between a *vector* dot product and the usual scalar product. A *vector* dot product involves a cosine factor: $\mathbf{a} \cdot \mathbf{b} = |\mathbf{a}| \cdot |\mathbf{b}| \cdot \cos\theta$. The θ is, of course, not the *phase* but the angle between the two vectors.

⁴² See: <u>Feynman's Lectures on Quantum Mechanics, Chapter 8, section 4</u>. The argument is quite dense and we, therefore, produced <u>one or two explanatory blog articles on it</u>. However, we will not repeat those here because <u>Caltech objected to us using some of Feynman's original material</u>.

⁴³ To be frank, we were actually *very* tempted to copy and discuss it here. It is quite instructive and intellectually challenging. However, we will leave it as an exercise for the reader to review Feynman's original lecture on this. Here, we will just identify the one *deus ex machina* moment in the argument—just in case the reader would not recognize it as such. After one or two pages of theory, Feynman introduces $U_{ij} = \langle i | U | j \rangle$ coefficients to describe the system (he does it for a *n*-state system, so we have states *i* or *j* = 1, 2, 3,..., *n*). These represent the 'time apparatus': the state may remain the same or go into another state as time passes by and so that is what the *n*×*n* matrix, *operator*, process or whatever you want to call it describes. Now, we have all of the coefficients C_i that describe the amplitude to be in state *i*. These are functions of time and so we should think of their time derivatives (yes, the differential equations are round around the corner now). Feynman thinks of the time derivatives in terms

result:

$$i\hbar \frac{dC_1}{dt} = H_{11}C_1 + H_{12}C_1$$

$$i\hbar \frac{dC_2}{dt} = H_{21}C_1 + H_{22}C_1$$

You may wonder: what *is* this? It does *not* define those Hamiltonian coefficients H_{ij} , does it? The answer is: it actually does.⁴⁴ We must move and so we will not dwell on this.⁴⁵ The coefficients C_1 and C_2 vary in time and to find them, we must solve for these Hamiltonian coefficients, which relate the $C_1(t)$ and $C_2(t)$ functions to their (time-)derivatives. These Hamiltonian coefficients are *not* time-dependent: they are constants and one can show they are related to the *energy* levels and/or the energy difference between them. To be precise, one can show⁴⁶ that, in this particular case, the coefficients in the Hamiltonian will be equal to:

of (infinitesimally small) *differentials* and, hence, writing something like this makes sense (we know we are *terribly* abstruse here—just check out <u>Feynman himself</u> for the nitty-gritty):

$$C_i(t + \Delta t) = \sum_j U_{ij}(t + \Delta t, t)C_j(t)$$

The $U_{ij}(t+\Delta t, t)$ element is a differential itself, and the next step in the argument (you are probably totally lost now but we are getting to the Hamiltonian here) is to write it as the following first-order approximation:

$$U_{ij}(t + \Delta t, t) = \delta_{ij} + K_{ij}\Delta t$$

This is all a bit mysterious, but so far so good. Feynman's deus ex machina move is to replace the K_{ij} coefficients by "taking the factor $-i/\hbar$ out of these coefficients." He writes he does "for historical and other reasons" but, of course, this is the point at which he actually uses the Planck-Einstein relation to define natural time units: why suddenly divide by \hbar otherwise? It is surely *not* an innocent operation.

Not only does it introduce Planck's constant – totally out of the blue! – but it also inserts the imaginary unit (i) in what turn out to be differential equations. It, therefore, totally changes the character of their solutions: we will get the periodic functions we need, so it works (of course, it does)—but it is *plain illegal* from a logical point of view. Any case, we cannot dwell on this here. To make a long story short, Feynman re-writes the above as:

$$U_{ij}(t + \Delta t, t) = \delta_{ij} - \frac{i}{\hbar} H_{ij} \Delta t$$

Re-inserting this expression in the very first and some re-arranging then gives the set of differential equations with the Hamiltonian coefficients you are probably waiting for:

$$i\hbar \frac{dC_i(t)}{dt} = \sum_i H_{ij}(t) C_j(t)$$

This is the set of differential equations Feynman then uses for this two-state system too.

⁴⁴ See footnote 43. We get the Hamiltonian coefficients from a rather random substitution (not-so-random, I should say) of K_{ij} coefficients by $-i \cdot H_{ij}/\hbar$ coefficients in Feynman's 'time-machine equations'.

⁴⁵ If Feynman skips steps and logic, we can do so too.

⁴⁶ See the above-mentioned reference to Feynman's Chapter 8.

$$\begin{bmatrix} H_{11} & H_{12} \\ H_{21} & H_{22} \end{bmatrix} = \begin{bmatrix} E_0 & -A \\ -A & E_0 \end{bmatrix}$$

What this energy E_0 and the energy difference A actually means, should be clear from the illustration below, which shows what happens in the absence and/or presence of an external electric field.

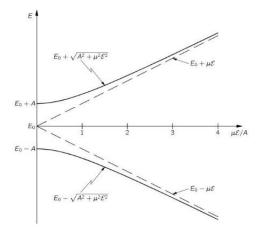


Figure 6: Separation of energy states when applying an external field⁴⁷

Indeed, **Figure 6** shows we can actually *not* talk of separate energy states if no external field is being applied: the energy of the ammonia molecule is just E_0 and there is no such thing as a higher or a lower energy state. In contrast, when an external field is being applied, we will have a higher or lower energy state depending on the position of the nitrogen atom and, therefore, of its position state. Feynman no longer refers to these energy states or levels as 1 or 2 but as state *I* and *II*, respectively. Why is that so? Because the nitrogen atom will no longer equally divide its time over position 1 and 2: if possible, at all, it will want to lower its energy *permanently* by *staying* in the lower energy state. This is, effectively, how we can *polarize* the ammonia molecules in a maser. Hence, the illustration below – which basically recopies **Figure 4** – is valid only for very small values of \mathcal{E}_0 : if we apply a stronger field, all ammonia molecules will align their dipole moment and stay aligned.

But so we will assume we are applying a very small field only—or no field at all, in which case we can calculate C_1 and C_2 as follows:

$$E_I = E_0 + \sqrt{A^2 + \mu^2 E^2}$$

 $E_{II} = E_0 - \sqrt{A^2 + \mu^2 E^2}$

In the absence of an external field (\mathcal{E} = 0), these formulas reduce to E₀ + A and E₀ – A, which correspond to the energy levels that are associated with the original $|1\rangle$ and $|2\rangle$ position states as well as with the C_1 and C_2 amplitudes, respectively.

⁴⁷ We gratefully acknowledge the online edition of Feynman's Lectures for this illustration too.

⁴⁸ We have no idea why Feynman thinks it is necessary to switch to a supposedly new set of *base* states, which he writes as $|I\rangle + |II\rangle$ respectively and which are associated with two new amplitudes C_I and C_{II} , respectively. It confuses the argument greatly and we do not see any added value. In any case, the reader should note **Figure 6** gives us the formulas for these two energy levels:

$$C_1 = e^{-i\frac{E_0}{\hbar}t}\cos\left(\frac{A}{\hbar}t\right)$$

$$C_2 = i \cdot e^{-i\frac{E_0}{\hbar}t} \sin\left(\frac{A}{\hbar}t\right)$$

How did we calculate that? We cannot say because we did not calculate anything here: we refer to Feynman for a rather ingenuous solution to that *set of differential equations* above.⁴⁹ The point is this: we can now take the absolute square of these amplitudes to get the probabilities:

$$|\mathcal{C}_1|^2 = \cos^2\left(\frac{A}{\hbar}t\right)$$

$$|C_1|^2 = \sin^2\left(\frac{A}{\hbar}t\right)$$

Those are the probabilities shown in **Figure 4**. The probability of being in state 1 starts at one (as it should), goes down to zero, and then oscillates back and forth between zero and one, as shown in that P_1 curve, and the P_2 curve mirrors the P_1 curve, so to speak. We can also see they respect the requirement that the sum of all probabilities must add up to 1: $\cos^2\theta + \sin^2\theta = 1$, always. That is Pythagoras' theorem once more.

Is that it? Yes. We must conclude our remarks here. We will do so by re-asking the question we started out with.

What is that we want to calculate?

We wanted to calculate that cycle time $\pi\hbar/A$, and so we did that. And then we did *not*, of course. We are still stuck with that circular $A = \mu \mathcal{E}_0$ equation. In fact, we need to ask ourselves: what determines E_0 ? At the very end of his argument, Feynman writes this⁵⁰:

"In the discussion up to this point, we have assumed values of E_0 and A without knowing how to calculate them. According to the correct physical theory, it should be possible to calculate these constants in terms of the positions and motions of all the nuclei and electrons. But nobody has ever done it. Such a system involves ten electrons and four nuclei and that's just too complicated a problem. As a matter of fact, there is no one who knows much more about this molecule than we do. All anyone can say is that when there is an electric field, the energy of the two states is different, the difference being proportional to the electric field. We have called the coefficient of proportionality 2μ , but its value must be determined experimentally. We can also say that the molecule has the amplitude A to flip over, but this will have to be measured experimentally. Nobody can give us accurate theoretical values of μ and A, because the calculations are too complicated to do in detail."

⁴⁹ Reference above: Feynman's Lectures, Volume III, Chapter 8, pages 8-11 to 8-14.

⁵⁰ To be truthful, it is not at the *very* end of his *exposé*—but just quite late in the game (section 9-2), and what follows does not give us anything more in terms of *first principles*.

This basically amounts to admitting defeat: we cannot calculate what we wanted to calculate based on *first principles*. Not a great success! In addition, we are still left with this great mystery: why do we need to take the (absolute) square of some complex-valued amplitude to get a probability?

Frankly, we would reverse that question: why would we calculate amplitudes by taking the square root of the probabilities?

Conclusions

We did not manage to clearly answer the question we started out with: what *are* those probability amplitudes, *exactly*? And why should we square them to get some probability? We cannot really answer this question because, while thinking of $C_1 \cdot |1\rangle$ and $C_2 \cdot |2\rangle$ as two vector *products*, we did *not* associate any mathematical function with $|1\rangle$ and $|2\rangle$. We therefore feel that we have just been blubbering around without being able to offer any real *interpretation* of what those probability amplitudes actually are: talking about these coefficients C_1 and C_2 without clearly stating what these $C_1 \cdot |1\rangle$ and $C_2 \cdot |2\rangle$ products represent results in the whole argument coming across as vague and mysterious. We think it is worse than trying to add apples and oranges but then we must assume that is how the author of the arguments we presented here – Richard Feynman – wanted it to be.⁵¹

We will try to come up with some better *definitions* of what a state or base vector might actually *be* here. We suspect it will depend on the specifics of the situation which, in this case, is the modeling of a maser: as long as long as we do not come up with a better description or definition of these state or base vectors, the concept of a probability amplitude is bound to remain as vague as the $|1\rangle$ and $|2\rangle$ notation that we have been using.

In the absence of such more precise description, we may just as well say we are looking at some oscillation here, and that we may use the Planck-Einstein relation once again to determine its frequency. The relevant energy to be used is an energy *difference* and the situation, therefore, resembles the energy difference between, say, two electron orbitals in the Rutherford-Bohr model of an atom. We write:

$$\omega = \frac{\Delta E}{\hbar} = \frac{2A}{\hbar} = \frac{2\mu E_0}{\hbar}$$

The particular form of the Planck-Einstein relation above may, therefore, be equivalent to a classical description of the situation at hand. Such simpler classical description has the added advantage that it avoids ill-defined concepts such as state vectors and probability amplitudes.

⁵¹ The reader may wonder why we single out Feynman here. The argument is more general, of course. If we have to reduce it somewhere, we should probably single out the inventors of state and amplitude math, so that's – chiefly – Erwin Schrödinger, Werner Heisenberg, Wolfgang Pauli, and Paul Dirac. We just have a bit of an argument with Feynman now because we are accused of referring to him too much. Otherwise, we generally like him: he did the best he could—taking into account the academic straitjacket he had to wear, of course!