Feynman's Time Machine

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Abstract

This paper discusses Feynman's famous derivation of the Hamiltonian matrix in his equally famous *Caltech Lectures on Quantum Mechanics*. We use Feynman's argument because it is very illustrative of the mainstream interpretation of what probability amplitudes may or may not represent. We refer to the argument as Feynman's Time Machine argument because the "apparatus" that is considered in the derivation is, effectively, the mere passage of time.

We show Feynman's argument is ingenious but, at the same time, very deceptive. Indeed, the substitution – for what Feynman refers to as "historical and other reasons" – of real-valued coefficients (K) by pure imaginary numbers ($-iH/\hbar$) effectively introduces the periodic functions (complex-valued exponentials) that are needed to obtain sensible probability functions. The division by Planck's quantum of action also amounts to an insertion of the Planck-Einstein relation through the backdoor. The argument is, therefore, typical of similar quantum-mechanical arguments: one only gets out what was already implicit or explicit in the assumptions. The implication is that two-state systems can be described perfectly well using classical mechanics, i.e. without using the concepts of state vectors and probability amplitudes.

This paper, therefore, complements earlier logical deconstructions of some of Feynman's arguments, most notably his argument on 720-degree symmetries – which we referred to as "the double life of -1" – as well as the reasoning behind the establishment of the boson-fermion dichotomy. This paper may, therefore, conclude our classical or *realist* interpretation of quantum mechanics.

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Introduction

To explain what a probability amplitude might actually *be*, one has to get into the specifics of the situation: explaining how a maser or a laser might work as opposed to, say, having a look at the polarization states of a photon, are two very different endeavors. However, despite the very different *physicality* of these systems, they allow for a similar approach in terms of their quantum-mechanical analysis.¹ The question is: why is that so?

The answer is: both phenomena involve periodicity and regularity – some *oscillation*, in other words – which can be *logically represented* by the same mathematical functions: a sinusoid or – what Nature seems to prefer – a combination of a sine and a cosine, i.e. an oscillation in two dimensions rather than one only, so that is Euler's $a \cdot e^{i\theta} = a \cdot (\cos\theta + i \cdot \sin\theta)$ function.²

The frequency of these oscillations is given by the Planck-Einstein relation: f = E/h. We should note the Planck-Einstein relation also gives us what we refer to as the *natural* unit for the system: its period T = 1/f = h/E.

When analyzing a maser or a laser, the energy E will be some energy *difference* between two *states*. This energy difference is measured with reference to some average energy (E_0) and is, therefore, usually written as 2A. The *period* of the oscillation is, therefore, given by³:

$$\mathbf{T} = \frac{1}{f} = \frac{h}{2A} = \frac{\hbar}{A}\pi$$

In order to ensure the probabilities slosh back and forth the way they are supposed to – which is as continuous functions ranging between 0 and 1 – we can present the probabilities of being in one or the other state (P₁ and P₂) as squared sine and cosine functions: P₁ = $\sin^2(2A \cdot t/\hbar)$ and $\cos^2(2A \cdot t/\hbar)$.⁴ The periodicity of these functions is effectively equal to π when measuring time in units of \hbar/A (**Figure 1**)⁵, and they also respect the normalization condition ($0 \le P \le 1$). Most importantly, Pythagoras' Theorem (or basic trigonometry, we'd say) also ensures they respect the rule that the probabilities must *always* add up to 1:

$$P_1 + P_2 = \sin^2(2A \cdot t/\hbar) + \cos^2(2A \cdot t/\hbar) = 1$$

³ The concept of an *angular* time period $(1/\omega = \hbar/A = T/2\pi)$ – the time *per radian* of the oscillation – is not in use but would actually be useful here: we will, in fact, use it as the time unit in the graph of the probabilities.

¹ The examples here (laser/maser and polarization of photons) are examples of two-state systems. However, our analysis will be valid for, or generalizable to, *n*-state systems. *A priori*, the analysis should, therefore, also be valid for $n \rightarrow \infty$ (i.e. for wavefunctions).

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.

⁴ The frequency in these functions is an *angular* frequency, which is why we have a factor 2: $\omega = 2A/\hbar \Leftrightarrow \omega \cdot t = 2A \cdot t/\hbar$.

⁵ The \hbar/A time unit is an *angular* time period $(1/\omega = \hbar/A = T/2\pi)$: see footnote 3.

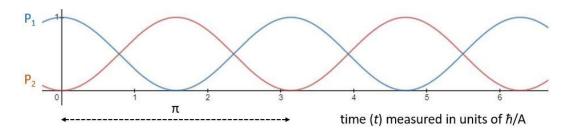


Figure 1: The probability functions for a two-state system

In fact, we do not see any other functional forms which would respect the above-mentioned conditions for *meaningfulness* in the context of defining probabilities.

We will now show how Feynman *smuggles*, so to speak, all of these functions and conditions into his argument when introducing the concept of probability amplitudes and constructing the Hamiltonian equations.

The maser as a two-state system

The two states of the ammonia molecule

While Feynman presents a general argument, he uses the maser as an example so as to focus ideas. We will, therefore, do the same.

The ammonia maser is one of the very first practical applications of the theory of quantum mechanics. It was built in the early 1950s (remember Feynman wrote his *Lectures* in the early 1960s) and its inventor, Charles Townes, wanted the *m* in *m*aser to refer to *molecular*. The mechanism is similar to that of a laser, which was invented a few years later: the *a*, *s*, *e*, *r* in *maser* effectively refer to the same as in *laser* (*a*mplification by *s*timulated *e*mission of *r*adiation).

However, instead of electromagnetic waves in the frequency spectrum of (visible) light, a maser produces microwave, radiowave or infrared frequencies. The latter are associated with *lower* energies, which correspond to the smaller *differences* between the energies that are associated with the *position* of the nitrogen atom in the ammonia (NH₃) molecule. The idea of the state may, therefore, be identified with the idea of the position of the nitrogen atom in the ammonia molecule (**Figure 2**).⁶

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.

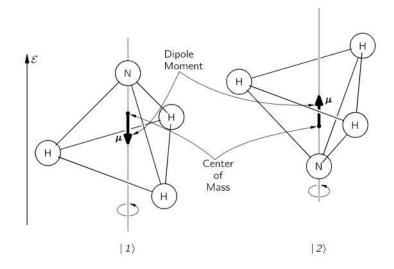


Figure 2: Ammonia molecules with opposite dipole moments in an electrostatic field⁷

The state concept

Figure 2 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* here or anything similar⁸, and one 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 way⁹ – 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 $\langle \chi |$. This is written in the way which will be familiar to the reader¹⁰:

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

⁸ As Feynman puts it, we assume all vibrational and rotational modes are exactly the same in the two states.

⁹ These changes are, in fact, at the heart of Feynman's argument—as we will see in a moment.

¹⁰ Note one needs to read this from right to left, like Arabic or Hebrew. We are not sure why Dirac chose this reverse order. It adds to the *magic*, of course, but it is a convention only.

Because this looks quite formidable, we should give a practical example as part of our discussion of the ammonia maser: if the electric field – the \mathcal{E} in the illustration¹¹ – 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.¹² 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.

What is the reference frame?

We should 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 NH₃ 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.¹³ This may seem to be a trivial philosophical remark but physicists sometimes seem to lose sight of this when doing more complicated abstract mathematical calculations.

We also need to make another philosophical 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 moment¹⁴ 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. One may think of it like this: the *valence* electrons allow the hydrogen to also (partly) fill its shell with paired electrons.

¹¹ We usually use *E* for an electric field but we use the \mathcal{E} symbol here so as to ensure there is no confusion with the E that is used to denote energy.

 $^{^{12}}$ 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.

¹³ 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 2**). 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.

¹⁴ All atoms with an uneven number of electrons have a magnetic moment because electrons in a *pair* (remember the standard configuration of an 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.

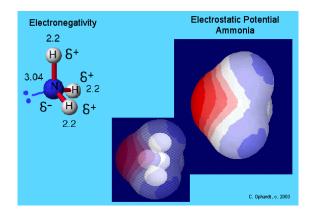


Figure 3: The charge distribution in an ammonia molecule¹⁵

We will let the reader *google* more details of the structure of this *system*.¹⁶ At this point, the reader 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!

We will not dwell on this. Just remember this when you are getting confused or if we would happen to be using non-specific language ourselves¹⁷: 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.

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, one needs 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 one should think of it in terms of *dynamics*. We modeled particles as *charges in motion*.¹⁸ 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

¹⁵ We gratefully acknowledge the source of this illustration: the <u>virtual Elmhurst College Chemistry Book</u>, Charles H. Ophardt, 2003.

¹⁶ 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 1*s* and 2*s* subshells have two, but the *three* 2*p* (subshells) each lack one electron, and then the 1*s* 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.

¹⁷ This inevitably happens when getting into quantum-mechanical descriptions so we will not apologize for it.

¹⁸ See our previous papers.

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*.¹⁹

Can we model this? Feynman did not think this was possible.²⁰ 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!²¹ We will, therefore, not dwell on this either: you should do your *PhD* on it!

The point is this: one 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.²²

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 – actually is.

Paraphrasing Wittgenstein²³, 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.²⁴ 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

¹⁹ 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.

²⁰ We will soon quote his remarks on this, *verbatim*, so be patient for the time being!

²¹ 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>

²² 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.

²³ We refer to Wittgenstein's theses in his *Tractatus Logico-Philosophicus*, which our reader may or – more likely – may *not* be familiar with.

²⁴ Of course, investigation may be useless because our measurement methods may *disturb* the system and, therefore, force it into one of the two states. We are probing one of the smallest of small things here, so *not* disturbing it will not be easy: measurement may, therefore, not be feasible from a *practical* point of view !

nitrogen atom, *in the absence of a measurement or polarization*, by thinking of it in very much the same way as we think of 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 revolutionary what we are doing here²⁵:

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 one 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 one should wonder: what *kind* of vectors are we talking about? Mathematicians refer to them as *Hilbert* vectors²⁶ and **Figure 4** shows why Schrödinger liked them so much: whatever they might represent, we can effectively add and multiply them, *somehow*.

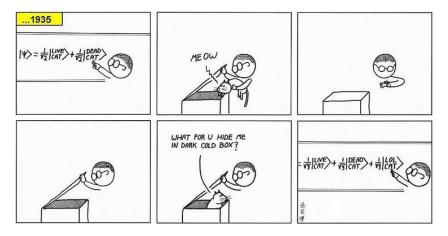


Figure 4: Adding cats or states? Adding them dead, alive or in-between?²⁷

²⁵ Some kind of *quantum leap*, we might say—but that would probably confuse the reader. ³⁰

²⁶ 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.*"

²⁷ 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 the box wears Schrödinger's glasses), the bra-ket notation was invented by Dirac. Schrödinger's seminal paper for the 1927 Solvay Conference (<u>La Mécanique des Ondes</u>) 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

It is really like adding apples and oranges. What do you get when you do that? Some fruits, right? (3) So we will talk about fruits but we should not forget the fruit consist of apples and oranges: that is the fruit menu of today, in any case (we might get grapes and bananas tomorrow).

The point is this: logic or logical states may be fuzzy, but *physical* states are *not*: the fruit is an apple or an orange—not something in-between. Likewise, the nitrogen nucleus is either here or there—not somewhere in-between.²⁸

2. So where are *we*? Yes. We were talking *physical* states. We multiply these with C_1 and C_2 in the $|\varphi\rangle = C_1 \cdot |1\rangle + C_2 \cdot |2\rangle$ formula: C_1 and C_2 are complex numbers (or complex *functions*, to be precise). Of course, because we are multiplying them with these state *vectors* – one may want to think of them as vectors too. That is not so difficult: complex numbers have a *direction* and a *magnitude*, so it is easy to think of them as vectors alright!²⁹

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. What does help is to think about what we are doing here—*logically* speaking, that is: we are using two *discrete physical states* to produce some new *logical state* which is defined by two complex-valued coefficients or – to be more precise – complex-valued *functions*. These functions will be well-behaved continuous functions.

Functions of what? Functions of time! To be precise, we will equate both of them with a complex-valued exponential function whose general shape is $C = a \cdot e^{-i \cdot \omega \cdot t}$.

One should note that all of these assumptions – which Feynman introduces rather casually – are *not* innocent: at this point, we are swapping the physics of the situation for some mathematical or logical representation of what might or might not be going on. If that is uncertainty, then it is *our* uncertainty—not Nature's! Hence, this $|\varphi\rangle$ state – which is the sum of the $C_1 \cdot |1\rangle$ and $C_2 \cdot |2\rangle$ states – is not a *physical* but a *logical* state: it exists in our mind only.³⁰ 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.³¹

modeled by wave mechanics—as opposed to matrix mechanics. It, therefore, bridges the two approaches, which complement each other, of course!

²⁸ At least not in a time interval that would be sufficiently large to be relevant! One should think of the time inbetween states as being too short to measure!

²⁹ We prefer such visualization or conceptualization to the idea of complex numbers being two-dimensional numbers. That is correct too, of course, but – perhaps – not so easy to visualize.

³⁰ 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.

³¹ We are not talking an apple-orange smoothie either!

Let us stop the philosophy here: let us now present Feynman's derivation of the Hamiltonian, which we refer to as his Time Machine argument—for reasons which will soon be clear.

Feynman's Time Machine

The objective of Feynman's rather convoluted argument is to calculate those C_1 and C_2 coefficients in the $|\phi\rangle = C_1 \cdot |1\rangle + C_2 \cdot |2\rangle$ formula. These coefficients are all that matters now: we do no longer care about how we can possibly represent the *physical* base states.³²

As mentioned above, we will equate both C_1 and C_2 with a complex-valued exponential function whose general shape is $C = a \cdot e^{-i \cdot \omega \cdot t}$. Feynman calls it 'trial' solutions to the set of differential equations he will develop but that should not mask the ruse: Feynman *imposes* these functional shapes in his argument. Why does he do that? It is because the derivative of a complex exponential – and of a real-valued exponential too, of course! – is an exponential function itself! So they make sense. Of course they do: there are actually no other solutions to the set of Hamiltonian equations we will derive, so it all comes as a package! Let us show how it works.

We write those coefficients C_1 and C_2 as functions of time, so we write them as $C_1(t)$ and $C_2(t)$. We will also have time derivatives $dC_1(t)/dt$ and $dC_2(t)/dt$. So far, so good. Now we get to the meat of the matter: Feynman's lecture on how states change with time³³ here makes for a great but rather complicated abstract logical argument which involves time as an apparatus. Feynman sums this up as follows:

"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 t₁ to time t₂."

After this introduction follows one or two pages of theory, in which 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 Feynman's '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 one would want to call it with the coefficients U_{ij} describes.

Now, we have all of the coefficients C_i that describe the amplitude to be in state i. These are functions of

[...]

³² Feynman makes the point quite explicitly by moving to another set of base states, which he denotes as *I* and *II*, as opposed to 1 and 2. These new base states are pure *logical* base states: they are also orthogonal and also observe other mathematical conditions so as to make sure we get the same well-behaved probability functions we want to get.

³³ We significantly abbreviate the argument here because we think Feynman makes it longer than it should be: <u>Feynman's Lectures on Quantum Mechanics, Chapter 8, section 4</u>. The extra whistles and bells in Feynman's argument probably serve to divert the reader's attention away from the various *deus ex machina* moves which, in sharp contrast to the sidekicks, remain largely *un*explained.

time and so we should think of their time derivatives.³⁴ Feynman thinks of the time derivatives in terms of (infinitesimally small) *differentials* and, hence, writing something like this effectively makes sense:

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

The $U_{ij}(t+\Delta t, t)$ element is a differential itself, and it is, obviously, a function of both t and Δt :

- 1. If Δt is equal to 0, no time passes by and the system will just be in the same state: the state is just the same state as the previous state. Why? Because there is no previous state here, really: the previous and the current state are just the same.
- 2. If Δt is very small but non-zero, then there is some chance that the system may go from state *i* to state *j*. Feynman models this by writing:

$$U_{ii}(t + \Delta t, t) = K_{ii} \cdot \Delta t$$

Feynman introduces yet another coefficient here: K_{ij} . Make no mistake about it: K_{ij} is a real-valued *proportionality* coefficient. It is just as real-valued as Δt and, therefore, as $U_{ij}!^{35}$

Of course, we should, somehow, incorporate the fact that, for very small Δt , the system is *more* likely to remain in the same state than to change. Feynman models this by introducing the Kronecker delta function. This all sounds and looks formidable but you will (hopefully) see the logic if you think about it for a while:

$$U_{ij}(t + \Delta t, t) = \delta_{ij} + K_{ij} \cdot \Delta t$$
$$\delta_{ij} = \begin{cases} 0 \text{ if } i \neq j \\ 1 \text{ if } i = j \end{cases}$$

The idea behind this formula is pretty much the same as that of using the first-order derivative for a linear (first-order) approximation of the value of a function $f(x_0 + \Delta x)$

$$f(x_0 + \Delta x) \approx f(x_0) + df = f(x_0) + f'(x_0) \cdot \Delta x = f(x_0) + \frac{df(x_0)}{dx} \Delta x$$

This is illustrated below (**Figure 5**). Feynman obviously uses Kronecker's δ_{ij} function to substitute for the function *f* in the formulas above, and so we should relate this to the probabilities. Indeed, the system is much more likely to have stayed in the same state (as opposed to going through a state change) if Δt is very small (probability close to 1), but more likely to change if more and more time goes by—so the probability to stay in the same state then goes down.

³⁴ The differential equations are, obviously, right around the corner now.

³⁵ Feynman carefully avoids any discussion as to whether we should think of the U_{ij} coefficient as being real- or complex-valued—and for good reasons: there is effectively no reason whatsoever to assume it should be complex-valued!

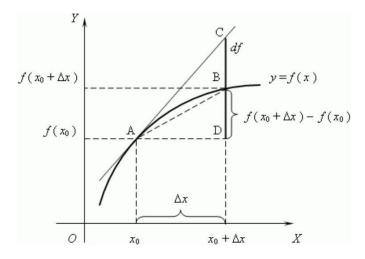


Figure 5: A first-order approximation of a function

We will not dwell too much on this—not because we don't want to but because you have to think all of this through for yourself in order to understand what we are writing here.³⁶ Just think about that proportionality with time:

$$U_{ii}(t + \Delta t, t) = 1 + K_{ii} \cdot \Delta t \ (i = j)$$
$$U_{ij}(t + \Delta t, t) = 0 + K_{ij} \cdot \Delta t = K_{ij} \cdot \Delta t \ (i = j)$$

The question this triggers, is really this: what are the relevant units here? We measure these 0 and 1 values *in what unit*, exactly? That question is answered by Feynman's grand *deus ex machina* move, and that is to replace these K_{ij} coefficients – simple *real-valued* proportionality coefficients – by "taking the factor –*i/ħ* out of these coefficients."³⁷

He writes he does so "for historical and other reasons"³⁸ but, of course, this is the point at which he actually uses the Planck-Einstein relation: why suddenly divide by \hbar otherwise?³⁹

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 equations which – by replacing the linear approximation with proper functions – will turn into a set of differential equations. As mentioned, the

³⁶ We did a few <u>blog posts on this</u>, but we should probably rewrite these to incorporate the more recent ideas we develop in this paper here. Kronecker's δ ij function

³⁷ We quote from the above-mentioned lecture (chapter 8 of Volume III of *Feynman's Lectures*, which have been made available online by Caltech.

³⁸He just says we should, of course, not confuse the imaginary unit *i* here with the *index i*. Jokes like this remind me of one of the books that was written on him: "*Surely You're Joking, Mr. Feynman!*"

³⁹ A sneak peek at the final solutions for our two-state system (the maser) tells us $H_{11} = H_{22} = E_0$ and $H_{12} = H_{21} = -A$. Needless to say, if we take the $-i/\hbar$ factor out of the K_{ij} coefficients, we should also take them out of the 0 and 1 terms. Also note that E_0 can be set to zero. It is just a matter of the reference point for the (potential) energy. Mathematically, it amounts to shifting the origin of the energy axis. Just substitute and see what makes sense (or not). One thing is for sure: there is a lot of hocus-pocus here—a lot of things that are implicit but are surely *not* innocent or merely 'historical reasons' only.

implicit insertion of the Planck-Einstein relation also fixes the (time) unit, which is just the reciprocal of the (angular) frequency A/\hbar .⁴⁰

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. Again, we will not dwell too long on this because we want the reader to think this through for himself. Hence, to make this rather long story short, we just note that Feynman re-writes the above as:

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

Re-inserting this expression in the very first and some more hocus-pocus⁴¹ and re-arranging then gives the set of differential equations with the Hamiltonian coefficients that you were probably waiting for:

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

This is the set of differential equations Feynman then uses for the two-state system representing the maser too. Indeed, for a two-state system, this is a set of two equations only:

$$i\hbar \frac{dC_1}{dt} = H_{11}C_1 + H_{12}C_1$$
$$i\hbar \frac{dC_2}{dt} = H_{21}C_1 + H_{22}C_1$$

These equations basically *define* the Hamiltonian coefficients H_{ij} in terms of the average energy E_0 and the energy *difference* between the two states and this average:

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

What this energy E_0 (note that this average energy can be set to zero⁴²) and the energy difference A actually means in the context of the particular system which Feynman used as an example – the maser – is illustrated below (**Figure 6**). It shows what happens to these energy levels in the presence of an external electric field ().

⁴⁰ See footnote 3.

⁴¹ The hocus-pocus here is, however, significantly less suspicious than the *deus ex machina* move when doing the mentioned substitution of coefficients!

⁴² See footnote 39.

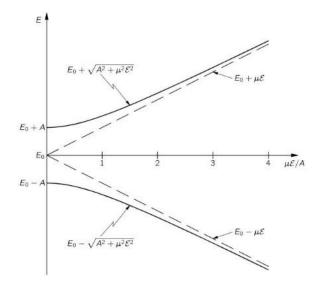


Figure 6: Separation of energy states when applying an external field⁴³

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 E₀ 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.

There is another thing we should mention here—something Feynman does not make very explicit either: when the external field becomes somewhat stronger, 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 illustrations above are 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.

In any case, assuming we are applying a *small enough* field only – or no field at all – we can solve the equations and calculate C_1 and C_2 as follows:

$$C_{1} = e^{-i\frac{E_{0}}{\hbar}t}\cos(\frac{A}{\hbar}t)$$
$$C_{2} = i \cdot e^{-i\frac{E_{0}}{\hbar}t}\sin(\frac{A}{\hbar}t)$$

How did we calculate that? We did not: we refer to Feynman here.⁴⁴ He introduces the mentioned socalled 'trial' solutions—which are *the* solution, of course! The point is this: we can now take the absolute square of these amplitudes to get the probabilities:

$$|C_1|^2 = \cos^2(\frac{A}{\hbar}t)$$

⁴³ We gratefully acknowledge the online edition of Feynman's Lectures for <u>this illustration</u> too.

⁴⁴ Reference above: Feynman's Lectures, Volume III, Chapter 8, pages 8-11 to 8-14.

$$|C_2|^2 = \sin^2(\frac{A}{\hbar}t)$$

Those are the probabilities shown in **Figure 1**. 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. As mentioned also, it is quite obvious they also respect the requirement that the sum of all probabilities must add up to 1: $\cos^2\theta + \sin^2\theta = 1$, *always*.

Is that it? Yes. We have been too long already and so we must conclude our paper here. We will do so by asking the question we should have started with.

What is that we want to calculate?

We wanted to calculate that cycle time $\pi\hbar/A$ (or the related frequency), and so we did that. And then we did *not*, of course—because all of the above uses an $A = \mu \mathcal{E}_0$ equation. We talked about the dipole moment (μ), but not about \mathcal{E}_0 . So how do we get \mathcal{E}_0 ? How do we *calculate* it?

The answer is: we don't calculate it. No one does. Its value must be related to the strength of the external field \mathcal{E} , but what field are or should we be applying here? Feynman is rather vague about that, but we get some kind of answer in his next lecture.⁴⁵ It turns out that, when actually operating an ammonia maser, we will apply an electric field 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. This field is this:

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

$$\omega = \omega_0 = 2A/\hbar$$

The question now becomes: what is that resonant frequency? This is, effectively, a circular argument: we define A in terms of μ and \mathcal{E}_0 , and vice versa! In fact, we need to ask ourselves this: what determines E_0 ? There is no conclusive *theoretical* answer to that question: it is, apparently, just something we measure experimentally. Indeed, at the very end of his argument, Feynman writes this⁴⁶:

"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

⁴⁵ Chapter 9 of Vol. III, which deals with the ammonia maser specifically, as opposed to just mentioning what is needed for this heuristic derivation of the Hamiltonian matrix (Chapter 8).

⁴⁶ 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*.

experimentally. Nobody can give us accurate theoretical values of μ and A, because the calculations are too complicated to do in detail."

This, then, amounts to admitting defeat: we cannot calculate what we wanted to calculate based on *first principles*. Not a great success!

Conclusions

We solved many mysteries in this paper – by highlighting the circularity (and/or plain deceit) in Feynman's quantum-mechanical arguments – but we are still left with one question: 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 and how can we calculate amplitudes by taking the square root of the probabilities? Why does it all work out? Why is it that the amplitude math mirrors the probability math? Why can we relate them through these squares or square roots when going from one representation to another?

The answer to this question is buried in the math too, but is based on simple arithmetic. Note, for example, that, when insisting base states or state vectors should be orthogonal, we actually demand that their squared sum is equal to the sum of their squares:

$$(\boldsymbol{a} + \boldsymbol{b})^2 = \boldsymbol{a}^2 + \boldsymbol{b}^2 \Leftrightarrow = \boldsymbol{a}^2 + \boldsymbol{b}^2 = \boldsymbol{a}^2 + \boldsymbol{b}^2 + 2\boldsymbol{a}\cdot\boldsymbol{b} \Leftrightarrow \boldsymbol{a}\cdot\boldsymbol{b} = 0$$

This is a logical or arithmetic condition which represents the physical condition: two physical states must be discrete states. They do not overlap: it is *either* this *or* that. We can then add or multiply these physical states – *mix* them so as to produce *logical* states, which express the uncertainty *in our mind* (not in Nature!) – because these base states are, effectively, independent. That is why we can use them to construct another set of (logical) base vectors, which will be (linearly) independent too! It is only because of the *physics* behind.⁴⁷

The more fundamental point is this, however: **we can spare ourselves the trouble of calculating amplitudes!** We can, just as well, say that we are looking at some *classical* oscillation here and that – as usual – we can use the Planck-Einstein relation 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. The following equation is, therefore, quite self-evident:

$$\omega = \frac{\Delta E}{\hbar} = \frac{2A}{\hbar} = \frac{2\mu \mathcal{E}_0}{\hbar}$$

Such simpler classical description does not need any ill-defined concepts such as state vectors and probability amplitudes. Nor does it need convoluted arguments to calculate functions that have no real meaning.

⁴⁷ If there is something you remember from vector algebra, it should be : one has to choose an unambiguous *origin* for the vector space. The *physicality* of the situation we are modeling has a similar significance here.