Lectures on Physics Chapter IV : Electron Propagation in a Lattice

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Abstract

We apply our realist interpretation of quantum mechanics to an analysis of the mechanics of electron propagation through a crystal and derive a formula for the *effective* mass of an electron which differs by a factor 2 from Feynman's. We think this solves his rather weird remark on the relation between the effective and free-space mass of an electron, which says the effective mass turns out to be 2 to 20 times the free-space mass of the electron. Our calculations imply the effective mass equals the free-space mass in the absence of a potential barrier between successive atoms in an lattice, which is what is to be expected. We also find Feynman's use of the small angle approximation for the argument of the wavefunction (so as to simplify the energy formula) is unjustified: the order of magnitude of the kb factor in the energy formula is one *rad* (radian), so that is too large for an small angle approximation. This remarkable result is surprising but makes sense because the reduced energy formula has no maximum, which contradicts the empirical reality of the conduction band in conductors as well as in semiconductors.¹

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¹ As for the title of this paper, we wrote a few which we jokingly numbered just like Feynman's famous <u>Lectures on</u> <u>Quantum Physics</u> for the freshman and sophomore classes at Caltech (1963). Unlike some what might think, they are *not* a re-write. They amount to what we refer to as <u>a realist interpretation of quantum physics</u>. However, we do re-use some of the illustrations and, of course, the formulas are the formulas: we just *interpret* their meaning very differently. In fact, we actually *give* many of the quantum-mechanical equations a meaning beyond the math. To paraphrase <u>Sabine Hossenfelder</u>, we like to think we are one of the few who do *not* get 'lost in the math.'

Electron Propagation in a Lattice

Introduction

Feynman's lectures on how an electron – or an excitation or some other irregularity² – might move through a one-, two- or three-dimensional array of atoms (a *lattice*, in other words³) yield sensible formulas – with a formula for the conduction band as the key result – but, even after multiple readings, still leave one rather bewildered. We do feel his treatment of the matter suffers from some imprecision in the concepts and, at times, rather chaotic heuristic arguments. In fact, despite Bill Gates's praise of Feynman as "the best teacher" he never had⁴, Feynman's treatment of the matter⁵ reminds us of John P. Ralston's self-criticism: "Quantum mechanics is the only subject in physics where teachers traditionally present haywire axioms they don't really believe, and regularly violate in research."⁶ Let us try to do better by exploring possible definitions of the various concepts that are used, and also by injecting some *realism* in the description: what is that we are trying to talk about, *exactly*?

The results of Feynman's analysis can be summarized in one or two formulas, and so let us try to find out how we get these. We all know the formula for the energy band (which we will come back to in a moment) but the formula we want to *understand* – not in an approximate but in an *exact* way – is the formula for the (kinetic) energy of an electron as it is moves through the lattice:

$$E = E_v = \frac{1}{2}m_{\rm eff}v^2 = \frac{pv}{2}$$

with $m_{\rm eff} = \frac{p}{v} = \frac{\hbar k}{v} = \frac{\hbar^2}{2{\rm Ab}^2} \iff k = \frac{\hbar v}{2{\rm Ab}^2}$

The m_{eff} is the *effective* mass of the electron as it moves through the lattice. What other *variables* do we have here? The A and b are (given) *parameters* of the system (A is an amplitude, about which we will say more later, and b is the lattice spacing) so, yes, we basically need to explain m_{eff} , the (electron drift) velocity *v* and *k*, which is a wavenumber.⁷ So let us try to do just that.

² We deliberately avoid the use of terms like excitons or phonons for the time being – until we are ready to define them more precisely. We should note, however, that we will *not* be talking excitons or phonons in this paper: we will be discussing electron propagation only.

³ The term *crystal* is usual added (crystal lattice) to emphasize we are talking a *regular* or repetitive atomic or molecular structure, as opposed to say, a nuclear lattice. We think the context is clear enough. To better frame the discussion, the reader should think of semiconductor material: silicon or germanium crystals. Silicon (and germanium) atoms have four valence electrons, which they share in a diamond-like cubic cell structure. To be precise, carbon (C), silicon (Si), germanium (Ge), tin (Sn), and lead (Pb) all belong to the so-called <u>carbon group</u>. ⁴ <u>https://www.gatesnotes.com/Education/The-Best-Teacher-I-Never-Had</u>

⁵ We refer to Feynman's Lectures, Volume III, Chapter 13 and – to a much lesser extent – Chapter 14. We assume the reader is more or less familiar with them, if only because many modern textbooks basically copy Feynman's treatment of the subject – even if it was written in the early 1960s.

⁶ John P. Ralston, <u>How To Understand Quantum Mechanics</u>, 2017, p. 10-40. We cannot recommend the book because – to paraphrase <u>Sabine Hossenfelder</u> – Prof. Dr. Ralston quickly gets 'lost in math' too!

⁷ The wavenumber is often referred to as <u>spatial frequency</u> (its dimension is *radians per meter*) but, to interpret this term, we think it is easier to just present its basic relation to the more familiar concept of momentum and wavelength: $k = 2\pi/\lambda = 2\pi p/h = p/\hbar$. This is just the *reduced* form of the second of the two *de Broglie* relations, of

Feynman tells us that " m_{eff} has nothing to do with the real mass of an electron", although in "commonly used metals and semiconductors it often happens to turn out to be the same general order of magnitude, about 0.1 to 30 times the free-space mass of the electron."⁸ We do not agree with that. There must be *some* relation between the two mass concepts because, otherwise, the concept of a momentum ($p = m_{eff} \cdot v$) and a wavenumber $k = p/\hbar$ would not make any sense and should, therefore, not be used. Mass and energy are related through Einstein's mass-energy relation ($m = E/c^2$) but, of course, that is only the case if we have *all* of the energy, or the right concept of energy – potential, kinetic, or both?⁹ – so let us discuss the energy concept here.

We know the value of this (kinetic) energy of an electron is constrained to a band which is usually referred to as the conduction band.¹⁰ This band is defined by a minimum and a maximum energy level which Feynman writes as a function of some (average) energy level E_0 and some energy *difference* A (or 4A: we will discuss this 4-factor in a minute). The graph below (Figure 1) plots E as a function of the mentioned wave number $k = p/\hbar = m_{eff}v/\hbar = \hbar v/2Ab^2$. Needless to say, v is the (classical) velocity of the electron in material: quantum physicists think of it as a group velocity of a wave *packet*, but we think it is the actual drift velocity of the pointlike electron.¹¹ As for b and A, b is the linear distance between two atoms (or molecules) in the array and A is... A requires some more explaining so, yes, let us finish the introduction and start.

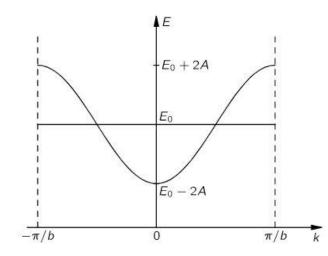


Figure 1: The energy band $E_0 - 2A \le E \le E_0 + 2A$ as a function of $k = p/\hbar = \hbar v/2Ab^2$

course $(h = p\lambda)$ which, in turn, is just the Planck-Einstein relation expressed in terms of (linear) momentum and wavelength. The first of the two *de Broglie* relations is the Planck-Einstein relation as we usually write it: $h = E/f = E \cdot T$. It may or may not help the reader to think of the Planck-Einstein relation as expressing Planck's quantum of action in two possible ways: (1) the product of energy and a cycle time $(h = E \cdot T)$ and (2) the product of momentum and a wavelength $(h = p \cdot \lambda)$. As such, the Planck-Einstein relation models nothing but a fundamental *cycle* in Nature. ⁸ Feynman's Lectures, Vol. III, p. 13-7. The original 1963 print edition talks about "real crystals" (instead of commonly used metals and semiconductors) and gives a range of "2 to 20 times the (free) electron mass."

⁹ We ask the question but do not answer it here because we want the reader to think about these questions without any prejudice for the time being. Indeed, we will be selling our 'mass without mass' model of an electron soon enough!

¹⁰ We will not distinguish between conductors and semi-conductors here, although it is probably easiest to think of semiconductor material here!

¹¹ See <u>our paper on de Broglie's matter-wave</u>.

The (i)A/ \hbar amplitude

A and b (and \hbar too, of course) are *given* constants, so the $k = p/\hbar = \hbar v/2Ab^2$ formula tells us k varies with the (electron) drift velocity v. What and how determines v? Feynman is totally vague about that. We should probably expect this drift velocity to vary with the voltage (potential difference) that is being applied, but let us think about this later. Also note we have a rather annoying 2 or 1/2 factor in the $k = \hbar v/2Ab^2$ formula. We have seen these 2 or 1/2 factors before but the reason it pops up this time seems to be more mundane: the energy difference in a simple two-state system is usually defined as the difference between an $E_0 + A$ and $E_0 - A$ level. Hence, the energy *difference* is usually defined as *twice* A, whatever A might represent. But - *Hey*! - we have an $E_0 - 2A \le E \le E_0 + 2A$ energy band here and, hence, an energy difference that is equal to *four* times that ubiquitous factor A. We are not sure why right now but we might find out later. So what *is* that factor A?

Feynman does not say all that much about it but he generously comes up with *some* clues, at least. He *defines* it as part of iA/\hbar , which is "the amplitude for the electron to jump from one atom to the next (per unit time)." He then simply states that: "There is not much more to be said about the various coefficients, such as the amplitude A, which appear in the theory. Generally they are very hard to calculate, so in practical cases very little is known theoretically about these parameters and for any particular real situation we can only take values determined experimentally."¹² It is, of course, a factor that must give us the actual *probability* of the electron going from here to there, but *how exactly?* The division by \hbar just *scales* the energy and gives us a value expressed per unit time. To be precise, it gives us – as per the Planck-Einstein relation – an angular frequency:

$$\mathsf{E} = h \cdot f = \hbar \cdot \omega \Longleftrightarrow \omega = \mathsf{E}/\hbar.$$

So this is to be written as $\omega = A/\hbar$ in this particular case. It reminds us of the (inverse of the) *cycle time* between two quantum-mechanical states. In fact, that is just what it is: $T = 1/f = 2\pi/\omega = 2\pi\hbar/A = h/A$. So here we may usefully remind the reader of Feynman's illustration of two probabilities 'sloshing back and forth', as he famously phrased it, as a function of time:

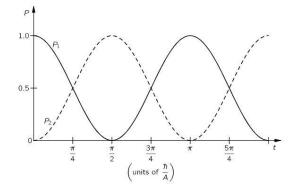


Figure 2: Probabilities sloshing back and forth¹³

¹² Feynman's *Lectures*, Vol. III, p. 13-2 and 13-9. It is customary to include the imaginary unit (*i*) in the amplitude, but we think this is not justified: the K_{ij} coefficients in the original Hamiltonian equations are real-valued numbers. Hence, you should think of this amplitude as a real-valued number: A/\hbar . Note its physical dimension again: it is some number *per second*. See our paper on <u>Feynman's Time Machine</u>, June 2020.

¹³ We gratefully acknowledge the online edition of Feynman's Lectures for <u>this illustration</u> too.

The graph measures time in radians, as opposed to seconds. Indeed, cycle times – in seconds, that is – are measured in units of *h*/A. It is a rather deep philosophical point which we could – but do not want to – enter into at this point of the narrative.¹⁴ The graph also triggers another obvious question: how do we *know* we are in state $|1\rangle$ at t = 0, π , 2π ,... as measured in the relevant unit here, which is \hbar /A? Or – what amounts to the same – how do we know we are in state $|2\rangle$ at $t = \pi/2$, $3\pi/2$,...?

[...] And? What is your answer?

[...] The answer is this: we do not. That is the point of quantum mechanics: we do not know – not exactly, at least. Quantum mechanics models statistical indeterminacy: we do not know the initial conditions and, therefore, we do not know when or how our electron is going to move from one state to another. The graph models probabilities, not realities! Let us get back to the problem at hand. We only gave you that graph and the talk on f = A/h or T = A/h so you have a better idea of what that amplitude A/\hbar actually *is*. So let us continue to try to say some more about that value A – some more than what the academic quantum physicists want to give us. What can it *be*?

We may assume the electron lowers it energy when joining an atom (or a molecule¹⁵) so as to create an ion.¹⁶ To move from one atom to another, it must, therefore, go through a potential barrier. This is nothing mysterious: potential barriers – or their corollary: potential wells – should not be thought of as static fields: they vary in time. They result from various charges moving around and creating 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 a temporary opening corresponding to a very classical trajectory in space and in time: think of it being in the right place at the right time – with one addition, perhaps: the *direction* of the (linear or angular) momentum needs to be right too.

Now, because we are modeling *regular* motion here – something with a cycle time (period) or, what amounts to the same, a frequency – we know the electron *must* move from one atom (or lattice cell) to another at *some* point in time: otherwise we would not be able to calculate these probabilities! Now that we are mentioning the calculation of probabilities, how does that work, *exactly*? Yes. Let us explain that by returning to the example of the two-state system before going back to our semiconductor.

We said we could not know for sure that the electron is in state $|1\rangle$ at t = 0, h/2A, h/A,...¹⁷ but the graph obviously assume we knew at point t = 0, at least! So how is *that* possible? I do not know. The most likely answer is that we had probably 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. But, again, we do not know *why* but the graph assumes we do! And then all is up in the air. Anything might happen! All we know is that the cycle time is equal to $\pi\hbar/A = h/2A$. Hence, we may expect the electron¹⁸ will have *swapped* from state $|1\rangle$ to

¹⁴ The reader might think we are joking, but we are not: our realist interpretation of quantum mechanics does think of matter-particles as material clocks: both time and distance can be measured in radians!

 $^{^{\}rm 15}$ It is usually an atom but molecular orbitals are theoretically possible too.

¹⁶ As you know, we may also have electron *holes*, in which case the ion is positive instead of negative.

¹⁷ We are measuring time in proper seconds now, rather than in units of \hbar/A . We do so by effectively multiplying 0, π , 2π , etc. by \hbar/A . For example, 2π becomes $2\pi\hbar/A = h/A$. It is always useful to recheck the physical dimension: h (or \hbar) is expressed in N·m·s, while A is an energy and, hence, is expressed in N·m. Hence, the division of h by A does yield seconds.

¹⁸ The smart reader will know that – in the case of Feynman's example of a two-state system (the maser) – we are actually *not* talking about an electron but about a nitrogen atom in a NH₃ (ammonia) molecule flipping back and

state $|2\rangle$ and then back again in the time interval h/2A. That is a full cycle. If we are interested only in it swapping from one state to the other, we may consider that to be the cycle, perhaps, and then the cycle time will be $\pi\hbar/2A = h/4A$. The *frequency* of swapping is just the inverse of the cycle time, of course: f = 1/T = 4A/h. Of course, academic quantum physicists will always write that as an *angular* frequency ($\omega = 2\pi f = 4A/\hbar$) and, just to confuse the uninformed reader and introduce even more mysterious quantum-mechanical language, they will call that the quantum-mechanical probability *amplitude* for the electron to swap states. As we will explain in a moment, the term *amplitude* is one of these terms which has several *different but related* meanings, so you should watch out!

Let us go back to the conduction band of our semiconductor: that factor 4 is no longer so annoying because, yes, an amplitude that is equal to $\omega = A/\hbar$ reads nicer than an amplitude that is equal to $\omega = 4A/\hbar$. So the factor 4 is there – it refers to a quarter (1/4) of a cycle – but you can choose where you put it: in your definition of the potential barrier (which is the conduction band, in this particular case) or in the definition of the amplitude.¹⁹

What about normalization? You may think this is normalized already, because it is *real*, and there is no reason to normalize reality, right? We rescale or normalize sizes and distances only because we want to express them in some different *unit*, but what is the point here? An amplitude is something *per unit time*, so its *value* is equal to the angular frequency. So that is *radians per second*. Very real. And we will multiply it, of course, with time, so we get the kind of dimensionless number that we want for an argument in a wavefunction.²⁰ So how can we relate this to the concept of probabilities or – to be precise – to probability *densities*? We need to take an absolute square somewhere, right? To be precise: we need to square the absolute value of a complex-valued amplitude or wavefunction, right? Right, but not here. It is, again, part of the utterly confusing language quantum physicists like to use to mystify things. As mentioned above, the concept of an amplitude may refer to related but very different things:

1. A complex-valued wavefunction which, for all practical purposes, can always be written as the product of a spatial and time-dependent part. So that is something like this²¹ – that ubiquitous 'trial solution' for a set of 'Hamiltonian equations'²²:

$$\psi(\mathbf{x},t) = a \cdot e^{i\theta} = a \cdot e^{i\left(\frac{\mathbf{E}\cdot t}{\hbar} - \frac{\mathbf{p}\cdot \mathbf{x}}{\hbar}\right)}$$

forth. It does not matter: we are talking something with *polarity* or some *charge* going back and forth through a potential barrier.

¹⁹ Thanks for *not* telling us these things, Mr. Feynman: I guess it is part of you challenging your students by not telling them everything, right? 😊

²⁰ Both the $(E/\hbar) \cdot t$ and the $(p/\hbar) \cdot x$ term in the argument of the wavefunction have no physical dimension: they are expressed in *radians* which, as we already briefly mentioned, may serve to both measure time as well as distance in our interpretation of matter-particles as physical clocks.

²¹ Having a plus or a minus sign in the (complex-valued) exponential ($e^{-i\theta}$) is a mere matter of *convention* for most physicists. We think that is a grave mistake: the plus or minus sign is related to the two possible *directions* of spin of a particle. See our paper on <u>Euler's wavefunction and the double life of -1</u>. We will also see the sign in front of the **p**·**x**/ħ term represents the direction of travel, which can be positive or negative. The plus or minus sign is, therefore, not random. That is also why we prefer to write **p**·**x** as a vector (dot) product.

²² If you want to know what they are, read our paper on <u>Feynman's Time Machine</u>.

2. The term amplitude may also refer to the (real-valued) coefficient in front of the complex exponential(s) in the wavefunction, so that is the *a* of the $a \cdot e^{i\theta}$ function.²³

3. The amplitude to go from one state to another, which is given by the fraction of (1) a cycle time (or half or a quarter of it) and (2) the time unit. So that is what we are talking about *right here and right now*.

So, yes, all of these concepts are effectively very different – but we need them all. The complex-valued wavefunction describes a state and is used in a system of Hamiltonian equations which describes all possible states. The amplitude to go from one state to another is a *related* concept but its nature is very different: it is like a probability. Indeed, you should note that the concept of a probability (usually) also involves some fraction of a period or a time unit: if we say that the probability of being in either of two states is 1/2, then we mean to say that it is in this or that state either of the two states about half of the time. Also, if we would know that the electron is in one of two possible states, then the probability of it going into the other state would be calculated as a function of (1) the time that has elapsed already, and (2) the (normal or average) cycle time. So, yes, it would involve that amplitude to go from one state to another!

Any case, we got sidetracked. Let us not worry about these concepts too much right now. We might come back to it. Let us continue to try to describe what might be happening in a semiconductor.

The elementary wavefunction

Planck's quantum of action (*h* or, in its reduced form, \hbar) models an elementary cycle in Nature. What is an elementary cycle? It can be anything: we think of an electron itself as an oscillating charge²⁴, a photon, a ring current in a superconductor is an oscillation too, an atomic or molecular orbital obeys the same law, an oscillation in a two-state system, etcetera. Regardless of the specifics of the situation, the frequency of these oscillations is always given by the Planck-Einstein relation: $E = h \cdot f \Leftrightarrow f = 1/T = E/h$.

The specifics of the situation here may look very different: we are, effectively, *not* looking at some stationary system here. Our electron moves, in either of two directions depending on the potential difference that is being applied. However, all motion is relative and so we might consider using relativity theory to analyze what may or may not be going on in the frame of reference of the electron itself.

Huh? Yes. Let us use a bit of relativity theory to analyze what may or may not be going on in the frame of reference of the electron itself.²⁵ Let us consider the idea of a particle (it is our electron, of course) traveling in the positive *x*-direction at constant speed *v*. This idea implies a pointlike concept of position: we think the electron will be *somewhere* at some point in time. The *somewhere* in this expression does not mean that we think the particle itself is dimensionless or pointlike. In fact, we think it is *not*. In this

²³ The informed reader will cry foul here: that coefficient may be complex-valued, right? Right, but there is always a way to write it as real-valued coefficient by moving the imaginary bit over to the time-dependent part of the wavefunction. See our paper on <u>the meaning of uncertainty and the geometry of the wavefunction</u>.

²⁴ We refer to <u>our interpretation of the *Zitterbewegung* theory</u> of an electron here, which we believe to be true because it explains all of the properties of an electron: its energy (and, hence, its equivalent mass), its magnetic moment (including the small anomaly which, therefore, is not an anomaly at all), and, last but not least, its angular momentum (spin).

 $^{^{25}}$ Just be patient and hang in there. It will be alright. If not, start again. 😊

particular case, we think of the electron as orbiting around a nucleus²⁶, so it takes up a rather large space. To be precise, the order of magnitude of the *radius* of this oscillation will be that of the Bohr radius of an atom, so that is about 150 times the electron's Compton radius.²⁷ Hence, the idea of position here only implies that we can think of some *center* of this oscillation, which we think of as being *physical*: a pointlike charge going round and round in a rather regular fashion (otherwise our idea of a cycle time and an orbital would not make no sense whatsoever). Hence, we have a *quantization* of space here but it is very different from, say, the quantization of space that results from applying the Planck-Einstein relation to the idea of a free pointlike charge (i.e. the *Zitterbewegung* or ring current model of an electron).

OK. We get this. Back to relativity. Back to the *motion* of our electron.²⁸ Two extreme situations may be envisaged: v = 0 or v = c. However, let us consider the more general case inbetween. In our reference frame²⁹, we will have a position – a mathematical *point* in space, that is³⁰ – which is a function of time: $x(t) = v \cdot t$. Let us now denote the position and time in the reference frame of the particle itself by x' and t'. Of course, the position of the particle in its own reference frame will be equal to x'(t') = 0 for all t', and the position and time in the two reference frames will be related by Lorentz's equations³¹:

$$x' = \frac{x - vt}{\sqrt{1 - \frac{v^2}{c^2}}} = \frac{vt - vt}{\sqrt{1 - \frac{v^2}{c^2}}} = 0$$
$$t' = \frac{t - \frac{vx}{c^2}}{\sqrt{1 - \frac{v^2}{c^2}}}$$

Hence, if we denote the energy and the momentum of the electron in our reference frame as E_v and $p = \gamma m_0 v$, then the argument of the (elementary) wavefunction $a \cdot e^{i\theta}$ can be re-written as follows³²:

²⁶ It is an *extra* electron so we have a negative ion instead of a neutral atom. However, this does not fundamentally alter the analysis. As you know, we might also model electron *holes*, in which case the ion is positive.

²⁷ We say 150 because that is close enough to the $1/\alpha \approx 137$ factor that relates the Bohr radius to the Compton radius of an electron. The reader may not be familiar with the idea of a Compton radius (as opposed to the Compton *wavelength*) but we refer him or her to the above-mentioned *Zitterbewegung* (ring current) model of an electron.

²⁸ We realize this may come across as an unnecessary digression, but we would not write it we think it was. So we leave it to the discretion of the reader to skip it or not.

²⁹ We conveniently choose our *x*-axis so it coincides with the direction of travel. This does not have any impact on the generality of the argument.

³⁰ We may, of course, also think of it as a position *vector* by relating this point to the chosen origin of the reference frame: a point can, effectively, only be defined in terms of other points.

³¹ These are the Lorentz equations in their simplest form. We may refer the reader to any textbook here but, as usual, we like Feynman's lecture on it (chapters 15, 16 and 17 of the first volume of Feynman's *Lectures on Physics*).

³² One can use either the general $E = mc^2$ or – if we would want to make it look somewhat fancier – the pc = Ev/c relation. The reader can verify they amount to the same.

$$\theta = \frac{1}{\hbar} (E_{\nu}t - px) = \frac{1}{\hbar} \left(\frac{E_0}{\sqrt{1 - \frac{v^2}{c^2}}} t - \frac{E_0 v}{c^2 \sqrt{1 - \frac{v^2}{c^2}}} x \right) = \frac{1}{\hbar} E_0 \left(\frac{t}{\sqrt{1 - \frac{v^2}{c^2}}} - \frac{\frac{vx}{c^2}}{\sqrt{1 - \frac{v^2}{c^2}}} \right) = \frac{E_0}{\hbar} t'$$

This is rather nice. We have just shown that the argument of the wavefunction is relativistically invariant: E_0 is, obviously, the rest energy and, because p' = 0 in the reference frame of the electron, the argument of the wavefunction effectively reduces to E_0t'/\hbar in the reference frame of the electron itself. However, you will say: this has nothing to do with the wavefunction of our electron in the lattice, right? Wrong.

Feynman's wavefunction for the electron in the lattice

We will not repeat Feynman's analysis here³³ but so he develops a system of Hamiltonian equations, and the challenge is to find the amplitude (or wavefunction) for the electron to be at some atom or position *n*. He writes these amplitudes as C₁, C₂,..., C_{n-1}, C_n, C_{n+1},... (you get the idea, right?) but we might as well write them as ψ_1 , ψ_2 ,..., ψ_{n-1} , ψ_n , ψ_{n+1} ,... Fancier, no? And guess what? Feynman shows these C_n or ψ_n functions must look like this:

$$e^{i[kx_n - \left(\frac{\mathbf{E}}{\hbar}\right)t]} = e^{-i\left(\frac{\mathbf{E}}{\hbar} \cdot t - \frac{\mathbf{p}}{\hbar} \cdot x_n\right)}$$

It is the same as the elementary wavefunction above. Not approximately, but *exactly*. The minus sign has got to do with the direction of travel, as Feynman readily acknowledges: "The wave can travel toward positive or negative *x* depending on the sign we have picked for *k*." We fully agree but, unlike Feynman, we actually think that wave *is* the electron or, at the very least, describes its motion very accurately.

Now, we should let that sink in some longer, so the reader should probably go for a coffee or smoke at this point in time, while we continue.

So far, so good, but we still do not have that formula for $k = p/\hbar = m_{eff}v/\hbar = \hbar v/2Ab^2$, right? Right. But we have a much better view on what is what now, and so we can see that there is no need to actually *explain k*: *k* is just the regular wave number, which we get from the second *de Broglie* relation.³⁴ What we need to explain is that formula for the effective mass:

$$m_{\rm eff} = \frac{p}{v} = \frac{\hbar k}{v} = \frac{\hbar^2}{2{\rm Ab}^2}$$

Let us first try to *read* it. The dimensional analysis comes out alright: $\left[\frac{\hbar^2}{2Ab^2}\right] = \frac{N^2 \cdot m^2 \cdot s^2}{N \cdot m \cdot m^2} = N \frac{s^2}{m} = kg.$

It also makes sense that m_{eff} is *inversely* proportional to A: if the amplitude for an electron to go from one atom to another is *large* – because the electron is only very loosely bound to the ionic atom so the potential barrier is very *low* – then the effective mass of the electron will appear to be *small*. And vice versa, of course.

³³ In case you would be doubting, we are still referring to Chapter 13 in Volume III.

³⁴ See footnote 7 or, if you do not trust us yet, the discussion of the *de Broglie* relations in <u>the Wikipedia article on</u> <u>the matter wave</u>.

But what about that b² factor? It is there because $x_n = n \cdot b^{35}$ and, when substituting that in the mentioned set of Hamiltonian equations, it gives us a formula for E and, therefore, for m_{eff}, which is the one we just wrote: $m_{eff} = \hbar^2/2Ab^2$. To be precise, it gives us the formula which is shown in Figure 1:

$$E = E_0 - 2A \cdot cos(kb)$$

What's E_0 ? It is the average of the maximum and minimum value of E. [...] We must be joking, right? No, we are not. The exact *values* of E and E_0 will depend on some reference point for the energy (the zero of energy, really) but E_0 itself is just the middle value between $E_0 + 2A$ and $E_0 - 2A$. Think about it!

So far, so good. Now how do we get that m_{eff} formula out of that energy formula? Feynman gets it through (1) the use of the small angle approximation for the cosine factor ($cos\theta \approx 1 - \theta^2/2$) and (2) choosing $E_0 - 2A$ as the zero of energy (or, what amounts to the same, *defining* E_0 as $E_0 = 2A$). The formula above then effectively reduces to:

$$E = E_0 - 2A \cdot (1 - k^2 b^2 / 2) = E_0 - 2A + Ak^2 b^2 = Ak^2 b^2$$

Is that legitimate? Let us first think about the second assumption³⁶: what *is* that energy E anyway? It is the *extra* energy which an electron gets *as it moves through the lattice*. The energy must, therefore, be *kinetic* (as opposed to potential), and we may effectively use the non-relativistic formula as an excellent approximation because we know those drift velocities are non-relativistic: we are talking like a millimeter per second, or even less. This may be surprising but it is what it is: the electric *signal* is lightning fast, but the electrons in the lattice themselves are covering very small distances only.³⁷ Hence, E is effectively E = $mv^2/2$ only, and we can now also understand Feynman's choice of the zero of energy: when v = 0, E will be zero. The *minimum* value for E must, therefore, be zero too! Hence, this is not just some random assumption: it is part and parcel of the *reality* of what we are modeling here.

OK. All of this is interesting, we hope (if only because we did not find such explanations in standard textbooks), so let us continue. We should, of course, note that we are still not sure whether or not we can apply that small angle approximation, but let us revisit that later. Let us first quickly re-check the logic of the $E = m_{eff}v^2/2 = Ak^2b^2$ and $p = \hbar k = m_{eff}v$ equations:

$$m_{\rm eff}v = \hbar \mathbf{k} \Leftrightarrow \frac{2\mathbf{A}k^2\mathbf{b}^2}{v} = m_{\rm eff}v \Leftrightarrow \mathbf{A}k^2\mathbf{b}^2 = \mathbf{E} = \frac{m_{\rm eff}v^2}{2}$$

The logic is OK but we still do not have that formula for m_{eff} because we do not have any formula for v either! So how can we *get* that? At this point, our *realist* interpretation of quantum mechanics differs again from Feynman's. Feynman calculates the velocity v by applying the formula for the *group* velocity of a wave *packet*:

³⁵ The b is the (linear) distance between two successive atoms: $x_{n+1} = x_n + b$ and x_0 is *defined* as $x_0 = 0$.

³⁶ We will devote a whole separate section to the other assumption (small angle kb so we can approximate). The analysis should surprise you – we think it is the most interesting bit of all! – so please keep reading.

³⁷ You can *google* this, or check <u>the Wikipedia article on drift velocities</u>. If you want an analogy, think of the musical chairs game but with the chairs on a line and all players agreeing to kindly move to the next chair for the new arrival and – importantly – the last person on the last chair agreeing to leave the game to get a beer. The *signal* moves fast, from start to end, but the persons themselves move only from one chair to the next.

$$v = \frac{d\omega}{dk} = \frac{d(\frac{E}{\hbar})}{dk} = \frac{d(Ak^2b^2)}{\hbar dk} = \frac{2Ab^2}{\hbar}k$$

We do not know where Feynman sees that wave packet, or why he needs it.³⁸ We do *not* see it. We see one wave, representing one particle. The only velocity that matters is the *phase* velocity, which is given by the simple ratio of ω and k:

$$v = \frac{\omega}{k} = \frac{Ak^2 b^2}{\hbar k} = \frac{Ab^2}{\hbar}k$$

The difference is a factor 2 or 1/2 again!³⁹ It gives a difference in the formula for the effective mass, of course. *My* formula does *not* have that factor 2:

$$m_{\rm eff} = \frac{p}{v} = \frac{\hbar k}{v} = \frac{\hbar^2 k}{Ab^2 k} = \frac{\hbar^2}{Ab^2}$$

Hence, my calculation of the effective mass gives a value which is twice that of Feynman:

$$m_{\rm eff} = \frac{p}{v} = \frac{\hbar k}{v} = \frac{\hbar^2 k}{2Ab^2 k} = \frac{\hbar^2}{2Ab^2}$$

Who is right? We think we are, of course! Why? Because we are convinced of what we have been writing so far, of course – which adds up to about 70 papers now!⁴⁰ However, Feynman himself seems to admit there is an issue here, because the original 1963 print edition of Feynman's Lectures says this:

"Don't forget that m_{eff} has nothing to do with the real mass of an electron. It may be quite different – although in real crystals it often happens to turn out to be the same general order of magnitude, about 2 to 20 times the free-space mass of the electron."⁴¹

Why 2 to 20 times, *exactly*? Why not 1 to 10, or some other more logical number? In our *realist* interpretation of quantum physics, m_{eff} *must* be related to the free-space mass of the electron and it must, therefore, be equal to 1 to 10 times (or more) the free-space mass of the electron – which it is according to our *phase* velocity formula. Right?

Maybe. Maybe not. Let us further explore the concept.

The concept of the effective mass of an electron

We casually introduced a lot of new ideas – a new *interpretation* of the quantum-mechanical model of conduction, basically – and we also conveniently simplified and made assumptions that were left unexplained. So perhaps it is time to recap. The assumptions are all quite reasonable assumptions –

⁴⁰ See: <u>https://vixra.org/author/jean louis van belle</u>.

³⁸ We are joking here, of course: Feynman has to see it because he has a linear conception of the matter-wave, just like *de Broglie*. See <u>our paper on the matter-wave</u>.

³⁹ We will not write about this here but, in most cases where we get this (a factor 1/2 or 2 in the calculations), it is because the energy concept is either kinetic or potential, but not both at the same time! Our oscillator model – the energy is the energy of a cycle in a two-dimensional oscillation – assumes kinetic and potential energy 'slosh back and forth' too. See <u>our paper on the meaning of the wavefunction</u>.

⁴¹ See footnote 8. We realize the reader may find this difficult to check, but we trust he or she will trust what we write here.

because they are the ones that are used (but left unexplained) by Feynman too. What about that energy concept, for example? In our (ring current) model of an electron, the energy is all of the energy – including the rest energy of the electron (we think of the rest mass of an electron as the inertia of the energy in the ring current and the electromagnetic field that sustains it). For the convenience of the reader, let us re-present the basic model, which we variously refer to as the *Zitterbewegung*, ring current or oscillator model of matter-particles (electrons and protons, basically⁴²).

We think of the (elementary) wavefunction $\mathbf{r} = \psi = a \cdot e^{i\theta}$ as representing the *physical* position of a pointlike elementary charge – pointlike but *not dimensionless*⁴³ – moving at the speed of light around the center of its motion in a space that is defined by the electron's Compton radius $a = \hbar/mc$. This radius – which effectively doubles up as the *amplitude* of the (elementary) wavefunction – can then be derived from (1) Einstein's mass-energy equivalence relation, (2) the Planck-Einstein relation, and (3) the formula for a tangential velocity, as shown below:

$$E = mc^{2} \\ E = \hbar\omega \} \Rightarrow mc^{2} = \hbar\omega \\ c = a\omega \Leftrightarrow a = \frac{c}{\omega} \Leftrightarrow \omega = \frac{c}{a} \} \Rightarrow ma^{2}\omega^{2} = \hbar\omega \Rightarrow m\frac{c^{2}}{\omega^{2}}\omega^{2} = \hbar\frac{c}{a} \Leftrightarrow a = \frac{\hbar}{mc}$$

This derivation⁴⁴ allows us to give a precise explanation of Prof. Dr. Patrick R. LeClair's interpretation of the Compton wavelength as "the scale above which the particle can be localized in a particle-like sense"⁴⁵, but we will limit ourselves here to an easy visualization of the model (Figure 3).⁴⁶

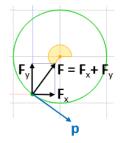


Figure 3: The ring current model of an electron

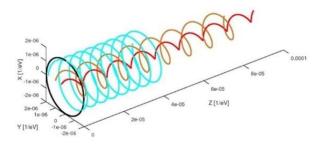
⁴² It may sound outrageous in light of various CERN experiments but, while we do believe in some kind of strong force (with a entirely different *geometry* than the electromagnetic force), we do *not* believe in the quark hypothesis!

⁴³ The *non*-zero dimension of the elementary charge explains the small anomaly in the magnetic moment which is, therefore, not anomalous at all. For more details, see our paper <u>on the electron model</u>.

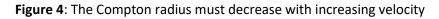
⁴⁴ It is a derivation one can also use to derive a *theoretical* radius for the proton (or for any *elementary* particle, really). It works perfectly well for the muon, for example. However, for the proton, an additional assumption in regard to the proton's angular momentum and magnetic moment is needed to ensure it fits the experimentally established radius. We shared <u>the derivation</u> with Prof. Dr. Randolf Pohl and the PRad team but we did not receive any substantial comments so far, except for the PRad spokesman (Prof. Dr. Ashot Gasparan) confirming the Standard Model does not have any explanation for the proton radius from first principles and, therefore, encouraging us to continue our theoretical research. In contrast, Prof. Dr. Randolf Pohl suggested the concise calculations come across as numerological only. We hope he will change his mind on this!

 ⁴⁵ Prof. Dr. Patrick LeClair, *Introduction to Modern Physics*, <u>Course Notes (PH253)</u>, 3 February 2019, p. 10.
⁴⁶ We refer, once again, to <u>our paper on the matter-wave</u> for an exploration of how all of this fits in with de Broglie's intuitions.

This *Zitterbewegung* (or ring current) electron may now move linearly and we may conveniently and without any loss on the generality of the argument choose our *x*-axis in our reference frame so it coincides with the direction of travel. We are then able to write its position *along the direction of linear motion* as a simple function of time itself: $x(t) = v \cdot t$. This combination of a pointlike charge *zittering* around some center and the oscillation as a whole them moving linearly is visualized below⁴⁷: the *radius* of the circulatory motion must effectively diminish as the electron gains speed.



Zitterbewegung trajectories for different electron speeds: v/c = 0, 0.43, 0.86, 0.98



We must, of course, immediately urge the reader to imagine the plane of oscillation to rotate or oscillate itself in line with our interpretation of the angular momentum vector \hbar as a vector rather than a simple scalar quantity. Also, when thinking of the electron moving linearly in an electromagnetic field, its precessional motion will yield a very different trajectory than the helical motion which is illustrated above. However, this does not alter the basic idea: we must think of the trajectory of an electron as a superposition of various motions – circular, orbital, linear and other, more complicated, patterns of motion in an electromagnetic field that varies in space and in time, perhaps.

However, we must keep things simple and so here we are considering the linear aspect only. So what is different here? Nothing much, perhaps. We put an electron in, and that is supposed to join the first atom, thereby *lowering* the joint energy of the system and, at the same time, ionizing it. In fact, we should probably be much more *real* and talk about silicon or germanium *crystals* jointly sharing their four valance electrons and, hence, we should probably be talking *molecular* rather than atomic orbitals here. But it is just a model, right? And so, yes, a lot is very different – *very* different – from our simple ring current model, but so we have to keep it as simple as possible and soldier on. So the illustration below (Figure 5) does capture the idea: the electron moves from one atom (or molecule or crystal cell) to the next, spends some time in an atomic or molecular orbital, and then moves on again. The signal travels fast, but the electron itself moves slowly – *very* slowly, it seems.



Figure 5: The idea of a moving electric signal in an atomic lattice

⁴⁷ We thank Prof. Dr. Giorgio Vassallo and his publisher to let us re-use this diagram. It originally appeared in an article by <u>Francesco Celani, Giorgio Vassallo and Antonino Di Tommaso</u> (*Maxwell's equations and Occam's Razor*, November 2017).

Why is so slow? The linear motion of the electron is really a 'stop-go, stop-go' motion, and we can now understand that the drift velocity consists of two very different components: the velocity in-between the moves, and the time it spends at stop:

- (1) The (average) time it spends at each stop is determined by that amplitude A; and
- (2) The time it spends inbetween depends on the velocity inbetween and the distance in between.

In short, that *phase* velocity which we calculated, makes sense⁴⁸, but may apply to the 'go' part of the motion only:

$$v_{phase} = \frac{\omega}{k} = \frac{Ak^2b^2}{\hbar k} = \frac{Ab^2}{\hbar}k$$

The critical question, of course, remains open: what is k? Ever since de Broglie wrote down his equations, it is *defined* as $k = p/\hbar$, and so that is what it is: the classical momentum of an electron. It *would be* equal to the free-space mass of an electron but, because we may not assume that the space between silicon or germanium crystals is, effectively, free space (it is filled with electromagnetic fields that vary in time and in space), we must write it as m_{eff}, so that's the concept of *effective* mass. However, contrary to what Feynman writes about it – "m_{eff} has nothing to do with the real mass of an electron" – it must, of course, be defined in terms of the free-space mass of an electron.

To be precise, the electron may travel more easily through the space inbetween, in which case the effective mass will be *less* than the free-space mass, or it may have to do some work *against* the electromagnetic fields, in which case the effective mass will exceed the free-space mass. Hence, while we were happy to write that the effective mass must be 1 to 10 times (or more) the free-space mass, we should correct ourselves. The text of the updated *Lectures* sounds good now:

"In commonly used metals and semiconductors it often happens to turn out to be the same general order of magnitude, about 0.1 to 30 times the free-space mass of the electron."⁴⁹

The small angle approximation for cos(kb)

We are now, finally, ready to answer the last and final question: is it *legit* to use the small angle approximation for the cosine factor ($cos\theta \approx 1 - \theta^2/2$) in the E = E₀ - 2A·cos(kb) formula so as to reduce it to E = E₀ - 2A· $(1-k^2b^2/2) = E_0 - 2A + Ak^2b^2 = Ak^2b^2$?

It *should* be, right? Why? Because Feynman says so. Sure. But let us *check* it, OK? Feynman really just babbles away about this question⁵⁰, but from what we write above, it is quite obvious this is an empirical question which we need to solve by looking at the order of magnitude of $k = p/\hbar$ and the lattice spacing b. So let us do that:

⁴⁸ Forget about Feynman's group velocity. That is inspired by an erroneous interpretation of what the matter-wave actually *is*: it is not linear, and so there is no need to superpose a finite or infinite number of matter-waves with slightly different frequencies and wavenumbers. One frequency (ω) and one wavenumber (*k*) will do. ⁴⁹ See footnote 8.

⁵⁰ He basically tries to show different values of *k* can represent "the same physical situation", which is a pretty disastrous strategy because then you have to *choose* one specific value to justify the small angle approximation, and so he does that by just "looking at what happens for small *k* – that is, when the variations of the amplitudes from one x_n to the next are quite slow" and then, *bam*, the E = Ak^2b^2 is there, and we should just take it for granted!

- 1. Typical velocities in atomic or molecular orbitals are of the order αc , with $\alpha \approx 0.0073$.⁵¹ Velocities go down as the inverse of the principal quantum number, so there is no inversesquare law here.⁵² Hence, we have an order of magnitude equal for the v in the p = mv equation in the range of 10⁶ m/s.
- 2. The effective mass is in the range of the free-space mass of an electron, so that is $10^{-30} \text{ N} \cdot \text{s}^2/\text{m}$.⁵³ The momentum p must, therefore, be of the order of $(10^6 \text{ m/s}) \cdot (10^{-30} \text{ N} \cdot \text{s}^2/\text{m}) = 10^{-24} \text{ N} \cdot \text{s}$.
- 3. We now divide by $\hbar = 6.62607015 \times 10^{-34}$ (an *exact* value since the revision of SI units last year⁵⁴) to get the order of magnitude for *k*. Check it: it must be a number like 0.15×10^{10} per meter. Yes, keep track of the physical dimension (and *meaning*) of everything! Of course, that looks *very* large instead of very small, but it is a rather typical order of magnitude for these wave numbers and we still need to multiply with b, remember?
- 4. The order of magnitude of the lattice spacing b is typically a few angstroms.⁵⁵ To be precise, the so-called *lattice constant* is about 5.431×10⁻¹⁰ m for silicon and 5.658×10⁻¹⁰ for germanium.

Hence, *k*b is a *number* of the order of... One!⁵⁶ *Huh?* Yes: 1. Not *exactly* one, of course – more like something like 0.3 or 1.5 or something. But that is the order of magnitude, indeed!

⁵¹ The velocity formula for Bohr orbitals is $v_n = \alpha c/n$, with n = 1, 2,... the principal quantum number (basically describing the energy level and the (rough) size of an orbital). Silicon has three shells, while germanium has four, so we may reasonably assume 1/n is going to be equal to 1/3 or 1/4.

⁵² The velocity formula for Bohr orbitals is $v_n = \alpha c/n$, with n = 1, 2,... the principal quantum number (basically describing the energy level and the (rough) size of an orbital).

 ⁵³ Electron mass (in kg) is 9.1093837015(28)×10⁻³¹ kg. Of course, to get the dimensions write, we need to use Newton's law to re-write mass as a measure of inertia, i.e. the equivalent of a force times an acceleration.
⁵⁴ In case you did not know or did not reflect about this 2019 revision of SI units, you should! I find it very interesting because it basically supports my interpretation of the Planck-Einstein relation as modeling *all* fundamental cycles in Nature!

⁵⁵ Feynman starts his lecture with noting this: "You would think that a low-energy electron would have great difficulty passing through a solid crystal. The atoms are packed together with their centers only a few angstroms apart, and the effective diameter of the atom for electron scattering is roughly an angstrom or so. That is, the atoms are large, relative to their spacing, so that you would expect the mean free path between collisions to be of the order of a few angstroms—which is practically nothing. You would expect the electron to bump into one atom or another almost immediately. Nevertheless, it is a ubiquitous phenomenon of nature that if the lattice is perfect, the electrons are able to travel through the crystal smoothly and easily—almost as if they were in a vacuum. This strange fact is what lets metals conduct electricity so easily; it has also permitted the development of many practical devices. It is, for instance, what makes it possible for a transistor to imitate the radio tube. In a radio tube electrons move freely through a vacuum, while in the transistor they move freely through a crystal lattice." [The italics are mine.] Of course, now you know he is writing a bit of nonsense here: it is not the electron that is traveling smoothly, easily or freely: it is the electrical signal, and - no ! - that is not to be equated with the quantum-mechanical amplitude. The quantum-mechanical amplitude is just a mathematical concept: it does not travel through the lattice in any physical sense ! In fact, it does not even travel through the lattice in a logical sense: the quantum-mechanical amplitudes are to be associated with the atoms in the crystal lattice, and describe their state – i.e. whether or not they have an extra electron or (if we are analyzing electron holes in the lattice) if they are lacking one. You may forget all of the formulas in this paper, but you should not forget this! 56 (0.15×10¹⁰)·(5.5×10⁻¹⁰) = 0.825. The 1/m and m dimensions obviously cancel out, so it is a real-valued number without physical dimension alright!

Of course, *k*b is expressed in *radians*, so we should think of that as an angle: an angle of 1 *rad* is about 60° (57.2958, to be precise). The point is: **this is** *not* **a small angle, and Feynman's use of the small-angle approximation is, therefore,** *not* **justified.**

How should we think of this? We think of it as a nice example of how our *realist* interpretation of quantum mechanics shows why and how mainstream quantum physics can fail to see how stuff actually works. The $E = Ak^2b^2$ formula was a bit of a joke anyway, wasn't it? It suggests anything goes, and that the concept of an energy band is basically not relevant. Why? Because an $E = Ak^2b^2$ energy formula models everything but a band, right? It has no upper limit, so that's not what reality tells us.⁵⁷

So... Well... What is the conclusion? Nothing much, but we will still devote a separate section to them (see below). Before we do so, we should note that we were very tempted to add another section about Schrödinger's wave equation for a linearly moving electron. However, we think we covered that – to a very reasonable degree, we think – in a previous paper on the matter-wave, amplitudes, and signals, so we will not dwell on it here.⁵⁸

Conclusion

This paper applied our realist interpretation of quantum mechanics to an analysis of the mechanics of electron propagation through a crystal. We derived a formula for the *effective* mass of an electron which differs by a factor 2 from Feynman's. We think this solves his rather weird remark on the relation between the effective and free-space mass of an electron, which says the effective mass turns out to be 2 to 20 times the free-space mass of the electron. Our calculations imply the effective mass equals the free-space mass in the absence of a potential barrier between successive atoms in an lattice, which is what is to be expected. We also find Feynman's use of the small angle approximation for the argument of the wavefunction so as to simplify the energy formula is unjustified. That makes sense because the reduced energy formula has no maximum, which contradicts the empirical reality of the conduction band in conductors as well as in semiconductors.

Jean Louis Van Belle, 2 November 2020

⁵⁷ Students may wonder what a maximum implies, really. Needless to say, if the applied voltage is too large, the potential difference will just rip the material apart. So that is end of story then. In that sense, then, there is neve a maximum, of course – but that is, of course, not what we are talking about here.

⁵⁸ See: <u>Matter-waves, amplitudes and signals</u>. The paper is quite long and, hence, the reader may want to skip several sections and jump to where he needs to jump.