The Meaning of Uncertainty and the Geometry of the Wavefunction

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Abstract

Uncertainty may result from (1) an impossibility to measure what we want to measure, or an impossibility to *observe* the system, (2) the limited precision of our measurement, (3) the measurement fundamentally disturbing the system and, as such, causing the information to be unreliable, (4) an uncertainty that is inherent to Nature. The latter position is referred to as the Copenhagen interpretation of quantum mechanics. We agree with Lorentz's and Einstein's viewpoint that there is no need to elevate indeterminism to a philosophical principle. The more important question is: how does quantum physics *model* it? How does it *deal* with it?

This paper wants to offer some thoughts on that and, in the process, highlights some contradictions which support Lorentz's (and Einstein's) position: we only have statistical indeterminism here and, hence, quantum physics is *not* a radical departure from classical physics. Hence, we will argue that quantum-mechanical uncertainty is nothing but statistical indeterminism. This is, effectively, the fifth interpretation of uncertainty which can be added to the list above, and we think it is the right one. We illustrate our position with a detailed discussion of the wavefunction(s) in the context of Schrödinger's wave equation for the hydrogen atom.

As we were getting into the nitty-gritty anyway, we also further explored the question in regard to the (possible) physical dimension of the real and imaginary part of the wavefunction. To paraphrase Feynman, we wonder what could be 'sloshing back and forth' between the real and imaginary part of the wavefunction? We think it is kinetic and potential energy. We, therefore, briefly present our two-dimensional oscillator model again, but using the metaphor of a multi-piston radial engine as a metaphor this time.

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The Meaning of Uncertainty and the Geometry of the Wavefunction

Introduction

Quantum mechanics is, essentially, a combination of Maxwell's equations and the Planck-Einstein relation. The Planck-Einstein relation gives us Planck's quantum of action, which appears to model an elementary oscillation: an electron is an oscillating charge, 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. Studying quantum physics is hard, *very* hard, because the formalism abstracts away from such specifics. We talk of quantum-mechanical states, but we abstract away from the *physical* reality underneath: we think of them as *energy* states only, but they must represent the system as a whole. The wavefunction must have all of the information on position and momentum (linear or angular): otherwise we would not be able to apply the relevant operators and get (average) values (or probabilities) for all of the *observables* (or *measurables*) out of it.¹

The main difference between classical physics and quantum physics is that, in quantum physics, we have only limited knowledge of the state of the system: there is uncertainty. The exact *nature* of this uncertainty is the subject of philosophical discussion. Uncertainty may result from:

- 1. An impossibility to measure what we want to measure, or an impossibility to *observe* the system: we might, perhaps, refer to this as an *Ungewissheit*.²
- 2. The limited precision of our measurement: this is what Heisenberg originally referred to as an *Ungenauigkeit*, i.e. before it became some metaphysical or epistemological principle.
- 3. The measurement might fundamentally disturb the system and, as such, cause the information to be unreliable.
- 4. The uncertainty is, perhaps, inherent to Nature. This philosophical position is referred to as the Copenhagen interpretation of quantum mechanics, and Heisenberg referred to it as the *Unbestimmtheitsprinzip*.

Bell's theorem is supposed to prove the latter position but a theorem depends on its assumptions – and these assumptions may be challenged. We basically agree with the remarks of the Dutch physicist H.A. Lorentz at the occasion of the 1927 Solvay Conference: there is no need to elevate indeterminism to a philosophical principle.³ The more important question is: how does quantum physics *model* it? How

¹ Physicists prefer the term observable: a physical quantity that can be measured. This definition shows we could also refer to it as a measurable. Both nouns have the same meaning.

² We did not check with the philosophers here, so our terminology suggestions are just what they are: suggestions. Words do not matter, but the distinctions might.

³ The full quote is this : "Je pense que cette notion de probabilité [Heisenberg-Bohr] serait à mettre à la fin, et comme conclusion, des considérations théoriques, et non pas comme axiome a priori, quoique je veuille bien admettre que cette indétermination correspond aux possibilités expérimentales. Je pourrais toujours garder ma foi déterministe pour les phénomènes fondamentaux, dont je n'ai pas parlé. Est-ce qu'un esprit plus profond ne pourrait pas se rendre compte des mouvements de ces électrons. Ne pourrait-on pas garder le déterminisme en en faisant l'objet d'une croyance? Faut-il nécessairement ériger l' indéterminisme en principe?"

does it *deal* with it? This paper wants to offer some thoughts on that and, in the process, highlights some contradictions which support Lorentz's (and Einstein's) position: we only have statistical indeterminism here and, hence, quantum physics is *not* a radical departure from classical physics. Hence, we will argue that quantum-mechanical uncertainty is nothing but statistical indeterminism. This is, effectively, a fifth interpretation which can be added to the list above, and we think it is the right one.

However, the more interesting question is whether or not we can show that quantum-mechanical amplitudes and the wavefunction⁴ – think of Schrödinger's equation and the solutions to it – have *physical* meaning. Can we do that? Let us try and see where we get.

Functions and physical dimensions

A dimensional analysis is always a good place to start, but what equations should we use? Feynman's canonical examples include the maser (the ammonia molecule as a two-state system), an electron moving in a lattice (*n*-state system modeling position), electron orbitals (Schrödinger's equation in a central field⁵), and many others. Where do we start? We will probably want to start from the simplest and let us, therefore, analyze the two-state system. In fact, our short list already triggers an obvious remark: the formalism of quantum mechanics talks about the states of system but, in practice, the state is often reduced to one *aspect* only: the position state, the momentum state, the energy state, etcetera. Using Dirac's bra-ket notation, we may formally write this as:

- --- $|x = n 1\rangle$, $|x = n\rangle$, $|x = n + 1\rangle$, etc. (position states in an *n*-state system⁶)
- $| \text{mom} = p \rangle$ (momentum state⁷)
- $| E = -E_R/n^2 \rangle$ (energy states⁸)

Hence, we should be cautious and, at each stage, clearly identify what *exactly* we are talking about. These states will all be represented by a complex-valued function (the wavefunction) or a complex number (a quantum-mechanical amplitude) but, *a priori*, we should expect that the *interpretation* of what the real and imaginary part of the wavefunction or amplitude might actually *be*, might depend on the situation at hand.

As we are talking terminology here, we should warn the reader for another potentially confusing thing: the term amplitude may refer to the complex number as a whole (let us, as per the convention⁹, write it

⁴ The two are not necessarily the same, and their meaning may also depend on the situation that is being modelled.

⁵ A central field depends on *r* only: the distance from the pointlike charge which, in the case of electron orbitals, is the nucleus (the proton inside of the hydrogen atom).

⁶ Think of a lattice on a line (a linear array of atoms or molecules).

⁷ The *mom* abbreviation is Feynman's, and the example here is *linear* momentum. If we are interested in the *direction*, we should probably write the momentum as a vector: **p**. We could also have given an example of an *angular* momentum state, in which case we should also distinguish between the magnitude and the *direction* of spin. Linear momentum is a polar vector (aka a true vector). Angular momentum is an axial vector (aka a pseudovector). Both are equally real – in a *physical* sense, that is.

⁸ The energies here are the energy levels of the *n*th orbital. E_R is the Rydberg energy (ionization energy).

⁹ The use of a plus or a minus sign for the *phase* ($+\theta$ or $-\theta$) in the complex exponential – hence, writing $e^{i\theta}$ or $e^{-i\theta}$ – is a matter of *mathematical convention*. In our papers, we have consistently argued the two mathematical possibilities may represent two *different* states: if, for some reason, the wavefunction would actually represent a physical rotation (of charge or whatever), then the two possibilities obviously represent opposite *spin* directions.

as $r = a \cdot e^{-i\theta}$) or to the coefficient in front of it (*a* only). Because the reader may doubt this statement, we will immediately give an example out of one of the more advanced models¹⁰: the wavefunctions for the state with an angular dependence to Schrödinger's equation for the hydrogen atom. These wavefunctions are written as¹¹:

$$\begin{split} \psi_{n,l,m} &= Y_{l,m}(\theta, \varphi) F_{n,l}(\rho) \\ \text{with:} \quad \rho F_{n,l}(\rho) &= e^{-\alpha \rho} \sum_{k=l+1}^{n} a_k \rho^l \\ \text{and:} \quad Y_{l,m}(\theta, \varphi) &= P_l^m(\cos \theta) e^{im\varphi} \end{split}$$

These wavefunctions are, in fact, only the *coefficient* of the actual wavefunction because the whole derivation is based on a separation of the time-dependent and the spatial part of the wavefunction. Somewhat confusingly, the same symbol (*psi*) is used to denote both, so the difference is only obvious when one writes the argument (independent variables) of the function in full:

$$\psi(\mathbf{r},t) = e^{-i\frac{\mathrm{E}}{\hbar}t}\psi(\mathbf{r}) = e^{-\frac{\mathrm{E}}{\hbar}it}\psi_{n,l,m}(\rho,\theta,\phi)$$

This all looks rather monstrous – it is ! – so let us break it down piece by piece. You should first note the switch from Cartesian coordinates $\mathbf{r} = (x, y, z)$ to polar (or spherical¹²) coordinates $\mathbf{r} = (\rho, \theta, \phi)$, because that is easier when talking circular or orbital motion.¹³ In addition, the distance from the center (the *radial* coordinate r) is now measured in a natural unit that goes with the system – the Bohr radius $r_{\rm B}$, to be precise¹⁴:

$$\rho = \frac{r}{r_B} = \frac{\alpha m_e c}{\hbar} r$$

As we are talking natural units, we may also note that, as per the Planck-Einstein relation ($E = \hbar \cdot \omega \Leftrightarrow \omega = E/\hbar$), the time-dependent part of the wavefunction ($e^{-\omega \cdot t}$) may be thought of as a clock ticking at the

$$r_B = \frac{\hbar}{\alpha m_e c} = \hbar \frac{2\mathcal{E}_0 hc}{q_e^2 m_e c} = \frac{4\mathcal{E}_0 \hbar^2}{m_e q_e^2} = \frac{\hbar^2}{m_e e^2}$$

Talking natural units, as part of solving the (Schrödinger wave) equation(s), Feynman also writes energies E in terms of the Rydberg energy: $E = E_R \cdot \epsilon$, with $E_R = \frac{\alpha^2 m_e c^2}{2} = \frac{q_e^4 m_e c^2}{8 \epsilon_0^2 h^2 c^2} = \frac{q_e^4 m_e}{2 \cdot (4\pi)^2 \epsilon_0^2 \hbar^2} = \frac{m_e e^4}{2\hbar^2}$. Hence, ϵ is like ρ , but it is used to measure energy.

 $^{^{10}}$ So we will *not* start with the simplest of models (the two-state system), then. $_{\odot}$

¹¹ We follow the notation from Feynman's *Lectures*, from which we borrow a lot of the material. We trust that the reader will be able to look up the original *Lectures* and distinguish between Feynman's formulas and text and our presentation and interpretation of it.

¹² Polar coordinates usually refer to a two-dimensional coordinate system, so a spherical coordinate system is then its three-dimensional version.

¹³ We still need to prove we are actually talking circular or orbital motion of some charge here, but we think the circumstantial evidence is fairly convincing.

¹⁴ We wrote the Bohr radius as a fraction of the Compton radius here. The reader can verify the substitutions, including Feynman's use of e^2 (the squared charge of an electron divided by $4\pi\epsilon_0$), by substituting the fine-structure constant (α) for its definition:

natural frequency of this oscillation.¹⁵ The (other) functions and symbols may be briefly explained as follows:

- --- The $F_{n,l}(\rho)$ function is a (finite) power series and is, obviously, just some real-valued function of the radial distance ρ .
- The P_I^m(cosθ) functions are known as the 'associated Legendre polynomials' (or functions). They
 are usually written in terms of derivatives of ordinary Legendre polynomials. We must refer the
 reader to readily accessible material here¹⁶

The $Y_{l,m}(\theta, \Phi)$ functions as a whole are known as the *spherical harmonics* (beautiful name, isn't it?) and they are a function of the polar and azimuthal angles θ and Φ .¹⁷ You should note that the $\psi_{n,l,m}$ amplitude (the *coefficient* of the actual wavefunction, really) would be real-valued, *always*, if we would not have that $e^{im\Phi}$ factor, which is equal to 1 (and, therefore, equally real-valued) if m = 0. And, of course, if we would multiply it through with the time-dependent part of the wavefunction ($e^{-i \cdot (E/h) \cdot t}$):

 $e^{-i \cdot (\mathsf{E}/\hbar) \cdot t} \cdot e^{i \cdot \mathbf{m} \cdot \Phi} = e^{-i \cdot [(\mathsf{E}/\hbar) \cdot t + \mathbf{m} \cdot \Phi]} = e^{-i \cdot (\omega \cdot t + \mathbf{m} \cdot \Phi)}$

Hence, this factor is just a phase *shift* and, therefore, should not matter at all in terms of the *physics* of the situation (it is just a matter of choosing our t = 0 point). So let us quickly look at that *quantum number*: what does it stand for? It is the *magnetic* quantum number, and it is usually denoted as m_z and referred to as the *z*-component of the angular momentum. This sounds very mysterious, and it is: *it is related to the weird 720-degree symmetry of the wavefunction which, in turn, results from mainstream academics not using the plus or minus sign of the imaginary unit to distinguish between the direction of spin.*

[...] You should read the latter phrase again, slowly. And because you will not understand what we are saying here, we talk about this in the annex. Here, we will just note what you know already: m is a number between -I and +I ($-I \le m_z \le +I$) and it gives us the (possible) orientations of the subshell. Here, we should quickly add that I is the quantum number that gives us the subshell within a given energy

¹⁵ We will let the reader think this through, and just remind him of the obvious formula for the cycle time (T): $\omega = 2\pi \cdot f \Leftrightarrow T = 1/f = 2\pi/\omega$. This shows the cycle time T is equal to $T = \omega/2\pi = E/2\pi\hbar = E/h$. The natural (angular) frequency is nothing but the natural time measured in *radians*: $\omega = 2\pi/T$. It is a somewhat weird idea to measure time in *radians* but, on the unit circle, the radian may be thought of as a natural distance as well as a natural time unit. It helps to literally think of an old-fashioned clock (with a hand for the seconds) ticking time away, with the tip of the hand doing the (circular) distance. Another, more abstract way, of thinking is this: we *count* the time in terms of the cycle of this oscillation (1, 2,..., n,...) but, if we would want to subdivide these cycles any further, we would divide them 2π (radians) rather than 12 (hours) or 60 (minutes or seconds).

¹⁶ The superscript m is an order number here: it is *not* an exponential. It is *not* a power of P_l, in other words. We used the <u>Wikipedia article</u> on these mathematical functions for more detail.

¹⁷ We use Feynman's notation here, and so he uses θ (*theta*) instead of some other letter (e.g. φ , *phi*) for the polar angle, which is slightly confusing because, in physics, θ is also used to denote the *phase* of the wavefunction, like in $\psi = e^{-\theta} = e^{-\omega t}$. Wikipedia says the *mathematical* convention is to use θ (*theta*) and φ (*phi*) for the polar and azimuthal angle respectively. Our *phi* (Φ) for the azimuthal angle is the capital letter *phi*. We may, therefore, use the lowercase *phi* (φ) if we would need to denote a phase, which is what we might do. As long as we know what we are talking about, it is all good, right?

state *n*. This *n* is the principal quantum number, and l = 0, 1, 2, ..., n - 1. Hence, if we have one energy state only, then we have only state: l = 0.¹⁸

What is the point? The point is that, when thinking about the *physics* of the situation, we can forget about that that $e^{im\Phi}$ factor. Think of it as being part of the time-dependent part of the wavefunction: we just shift the origin of time. That amounts to looking at the system – the *oscillation*, that is – a tiny bit earlier or later, and that does not matter because it is a perfectly regular oscillation. What we are interested in the *shape* of the *physical* orbitals, their energies, and other *physical* variables. Hence, for all practical purposes, we should think of the coefficient of our wavefunction – or the amplitude *sensu stricto*, or the spatial (position-dependent) part of the wavefunction, or whatever you want to call it – as a real number !

Is that important? Yes, it is. Knowing that a wavefunction – *any* wavefunction, really – can always be written as the product of a time-dependent and a spatial or time-independent function is huge, and it is equally huge to know that the time-dependent part will always look like $e^{-i\cdot\omega\cdot t + \varphi}$, and that the φ here is just some random phase shift which does not matter because we can always shift the t = 0 point however we would want to shift it: the physics of the situation won't change ! This is reflected in the fact that the absolute square¹⁹ of a complex exponential (when its coefficient *a* is 1, of course) is always equal to 1. We apologize for writing this out but it is, perhaps, good to remind ourselves of what a complex number really is: the vector sum of a sine and a cosine.

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

Let us continue our search of some *physical meaning* of the real and imaginary parts of the wavefunction by continuing our example.

What does it all mean?

Below we copy table 19.1 out of Feynman's Lectures, which gives us the *functional form* of those spherical harmonics: they combine sine and cosine functions. Now, we are interested in the *probability* to find the electron at point $\mathbf{x} = (x, y, z)^{20}$, and quantum mechanics tells us we can calculate these probabilities by taking the absolute square of the $\psi(\mathbf{x})$ wavefunction. To be precise, the theory of operators – and of the position operator, in particular – tells us the probability *density* $P(\mathbf{x})$ will be equal to $P(\mathbf{x}) = |\psi(\mathbf{x})|^2 = \psi(\mathbf{x}) \cdot \psi^*(\mathbf{x}) = \psi^*(\mathbf{x}) \cdot \psi(\mathbf{x})$, with $\psi^*(\mathbf{x})$ the complex conjugate of $\psi(\mathbf{x})$.²¹

¹⁸ We should refer to standard textbooks here, but we think our own presentation in our classical explanation of the Lamb shift has the advantage of (1) being succinct and (2) relating it to what we said on these weird 720degree symmetries vanishing if one would use the \pm sign in front of the imaginary unit to incorporate the two possible spin directions in the analysis straight from the start.

¹⁹ This term is a (slightly confusing, perhaps) shorthand for the square of the absolute value of a (complex- or realvalued) number. It is also referred to as the square of the *modulus* of the complex sum (sum of the real and imaginary part of the number).

²⁰ We have a bad habit of switching from r to x, or vice versa, for no reason whatsoever – except that you will find x is more common than r in the literature. A bold letter is a vector, in any case, and you may think r suggests we are working in polar rather than Cartesian coordinates, and vice versa.

²¹ The extension of quantum-mechanical ideas and formulas from one-dimensional space (a line) to three dimensions is not always as straightforward (Feynman, III-20-4) but, in this case, it surely is!

Orbital angular momentum, <i>l</i>	z- component, m	Angular dependence of amplitudes	Name
0	0	1	8
1	$\left\{ \begin{matrix} +1 \\ 0 \\ -1 \end{matrix} \right.$	$\leftrac{1}{\sqrt{2}} {\sin heta e^{i\phi}} \\ \cos heta \\ rac{1}{\sqrt{2}} {\sin heta e^{-i\phi}} ight\}$	p
2	$\left\{egin{array}{c} +2 \\ +1 \\ 0 \\ -1 \\ -2 \end{array} ight.$	$\left. \begin{array}{c} \displaystyle \frac{\sqrt{6}}{4} \sin^2 \theta e^{2i\phi} \\ \\ \displaystyle -\frac{\sqrt{6}}{2} \sin \theta \cos \theta e^{i\phi} \\ \\ \displaystyle \frac{1}{2} (3\cos^2 \theta - 1) \\ \\ \displaystyle \frac{\sqrt{6}}{2} \sin \theta \cos \theta e^{-i\phi} \\ \\ \displaystyle \frac{\sqrt{6}}{4} \sin^2 \theta e^{-2i\phi} \end{array} \right\}$	d
3		$\langle l,0 \mid R_y(heta)R_z(\phi) \mid l,m angle$	f
4	} {	$\propto Y_{l,m}(\theta,\phi)$	g
5	J	$\propto P_l^m(\cos\theta)e^{im\phi}$	h
÷			:

Figure 1: Spherical harmonics (source: Feynman III-19-3)

That gives us these wonderful *polar* graphs which, literally, depict the *shape* of those electron orbitals.²² We may note here that we are taking the square of the absolute value of a *real-valued* amplitude here. Hence, what matters is the magnitude only: positive or negative amplitudes give the same probability. Take, for example, the *p*-orbital (*l* = 1) for m = 0. The spherical harmonic is a simple $\cos\theta$ function and, yes, $|\cos\theta|^2 = \cos^2\theta = |\cos(-\theta)|^2 = \cos^2(-\theta)$.

So, yes, interpreting the math is not all that difficult. We are effectively talking the *physical* orbitals of the pointlike electron charge here, and the uncertainty is a mere statistical indeterminism. So it is really just like the propeller of that airplane: we do not know where it is, *exactly*, but we know it is always *somewhere*, at any given point in time. Please note this is *not* your usual crackpot interpretation of quantum physics. We may usefully quote Richard Feynman here:

"The wave function $\psi(\mathbf{r})$ for an electron in an atom does not describe a smeared-out electron with a smooth charge density. The electron is either here, or there, or somewhere else, but wherever it is, it is a point charge." (Feynman's Lectures, III-21-4)

²² To show we do google other textbooks from time to time, we refer the reader to <u>a chapter of a course (in physical chemistry) at the University of Michigan</u>: instructive, no hocus-pocus and good graphs.



Figure 2: Where is the propeller, exactly?²³

The rather primitive comparison with an airplane propeller triggers two more useful associations. One is the metaphor of an old-fashioned radial airplane engine, in which linear and circular motion come together (we will come back to this). The other is an analogy with the synchronization gear that was used in WW I for machineguns firing their bullets through the propeller: if there was no synchronization gear, some of the bullets would actually hit and considerably damage the propeller: the analogy with light (consisting of photons) going through a three-dimensional lattice with electrons in all kinds of orbitals readily comes to mind. We invite readers to also google scatter plots of electron position measurements for hydrogen and other atoms.²⁴

However, these reflections do not solve the question we started out with: what is the *physical meaning* of the real and imaginary parts of the wavefunction? Would they have a physical dimension, like a field – something like newton per coulomb (N/C), like the electric field, for example? In addition, Feynman's take on it leaves other interpretational issues: Schrödinger's orbitals imply the electron spends most of its time right on top of the proton, so how should we think of that? We could, perhaps, imagine some short-range repulsive force here but such solution would inject entirely new dynamics and, therefore, looks pretty unacceptable: assuming the electron, somehow, does go straight through the center or, else, bounces back – fully elastically, because momentum and energy should be conserved – is the only solution but raises other questions (which we will try to examine later, perhaps). Back to the question of a physical dimension for the wavefunction.

Should it have one? The argument is time and position – simple *numbers*, right? – so the wavefunction might just project these numbers onto a two-dimensional *mathematical* space only, right? Maybe. Maybe not. Could the operators give us a clue? Unfortunately not. Their physical dimensions are OK already²⁵:

²³ I downloaded this image from a website selling Christmas presents long time ago, and I have not been able to trace back from where I have got it. If someone recognizes this as *their* picture, please let us know and we will acknowledge the source or remove it.

²⁴ The above-mentioned <u>basic physical chemistry course of the University of Michigan</u> offers one, but here is <u>another one from Chemistry LibreTexts</u>.

²⁵ The energy operator – and the others as well, perhaps – depend on the problem at hand. The one here is derived from Schrödinger's wave equation for electron orbitals, so we basically continue the analysis for the very

- The energy operator $H = -\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r})$ comes with the $\frac{N^2m^2s^2}{m^2kg} + N \cdot m = \frac{N^2m^2s^2}{m^2\frac{Ns^2}{m}} + N \cdot m = N \cdot m$ dimension, so that is the physical dimension of energy alright.
- Likewise, the position operator x or and the momentum operator $P_x = -i\hbar \frac{\partial}{\partial x}$ come with the physical dimension of distance (m) and momentum $(\frac{N \cdot m \cdot s}{m} = N \cdot s)$ respectively.
- Finally, the angular momentum operator $L_z = x \frac{\hbar}{i} \frac{\partial}{\partial y} y \frac{\hbar}{i} \frac{\partial}{\partial z}$ comes with the $m \frac{N \cdot m \cdot s}{m} m \frac{N \cdot m \cdot s}{m} = N \cdot m \cdot s$ dimension, so that is, effectively the same as that of Plank's quantum of action itself (in reduced or non-reduced form).

Can we think of one that would suit the $P(\mathbf{x}) = |\psi(\mathbf{x})|^2$ equation? Probabilities or – to be precise – probability *densities* – should match energy or mass densities, right? Hence, we are talking kg/m³ or $N \cdot m/m^3 = N/m^2$, and we can now take a square root or something, right?²⁶ Correct, but note that the wavefunction here does *not* have the time-dependent part.²⁷ In fact, this wavefunction – the wavefunction for Schrödinger's electron orbitals – is a *real-valued* wavefunction: it is the amplitude *sensu stricto* and, hence, talking of the meaning of the real or imaginary part of this wavefunction makes no sense: there is only a real part to it. If we want to talk about the whole thing, then we should put the time-dependent part (the complex-valued function that gives the whole its real and imaginary mathematical dimension) back in.

So, again, what are we talking about, then?

The oscillator model

We have been thinking about these things for a while now, and we have no definite answer. However, the interplay between the real and imaginary part of the wavefunction reminds one of these probabilities 'sloshing back and forth', as Feynman would say, as a function of time in a simple two-state system. So what would slosh back and forth between the real and imaginary part of the wavefunction? We see one obvious candidate – to be truthful: we do not see any others – and that is kinetic and potential energy. Here we need to revive, perhaps, our two-dimensional oscillator model, but extend it from circular orbitals to orbitals with fancier geometric shapes, such as those in Schrödinger's model of an atom, indeed!

same problem at hand. Note that the symbols used for operators vary (with or without hat or special script). Ours are probably too simple.

²⁶ Note that we can often switch from energy to mass units and vice versa without too much trouble, but units matter here, and kg/m³ or J/m³ are different units. The physical dimension of the c^2 in the mass-energy equivalence relation (E = m c^2) matters here. It is *not* just some constant. Converting kg to N·s²/m units yields the kg/m³ = N·s²/m⁴ unit. We have no idea what we could possibly do with that. In contrast, the N/m² is much more natural: force per unit surface. Easy, right?

²⁷ The reader should also carefully check on what the listed operators are operating on: as mentioned, physicists often conveniently forget about the time-dependent when doing their math. It is usually *not* a problem but when trying to carefully *interpret* what is what – as we are trying to do here – it is.

Let us briefly recap the metaphorical idea.²⁸ If we combine *two* oscillators in a 90-degree angle – think of two springs or two pistons attached to some crankshaft²⁹ – then we get some *perpetuum mobile* which stores *twice* the energy of a single oscillator, and the motion of the pistons will reflect that of a mass on a spring: it is described by a sinusoidal function, with the zero point at the center of each cylinder. We detailed the math elsewhere³⁰ and only note the model is relativistically correct. Indeed, the relativistically correct force equation for *one* oscillator is:

$$F = dp/dt = F = -kx$$
 with $p = m_v v = \gamma m_0 v$

The energy conservation equation can be derived from multiplying both sides with v = dx/dt. One can then verify the following³¹:

$$v\frac{\mathrm{d}(\gamma m_0 v)}{\mathrm{d}t} = -\mathrm{kx}v \Leftrightarrow \frac{\mathrm{d}(\mathrm{m}c^2)}{\mathrm{d}t} = -\frac{\mathrm{d}}{\mathrm{d}t} \left[\frac{1}{2}\mathrm{k}x^2\right] \Leftrightarrow \frac{\mathrm{d}E}{\mathrm{d}t} = \frac{\mathrm{d}}{\mathrm{d}t} \left[\frac{1}{2}\mathrm{k}x^2 + \mathrm{m}c^2\right] = 0$$

For the potential energy, one gets the same $kx^2/2$ formula one gets for the non-relativistic oscillator. That is no surprise: potential energy depends on position only, not on *velocity*, and there is nothing relative about position. However, the $(\frac{1}{2})m_0v^2$ term that we would get when using the non-relativistic formulation of Newton's Law is now replaced by the $mc^2 = \gamma m_0 c^2$ term. Both energies vary – with position and with velocity respectively – but the equation above tells us their *sum* is some constant. Hence, the game with two oscillators working in tandem should work here too.³² In addition, the analogy can be extended to include two *pairs* of springs or pistons, in which case the springs or pistons in each pair would help drive each other. Even more interestingly, we may imagine a multi-piston *radial* engine (Figure 3)³³.

²⁸ These ideas will probably intrigue us for the rest of our life, and we are not sure if we will ever get beyond metaphorical ideas only in regard to these deep questions.

²⁹ Academics seem to prefer springs, but I like engines. In fact, the metaphor was inspired by a discussion with my son on the efficiency of a Ducati engine, which effectively has a 90-degree bank angle. The 90° angle of the V-2 makes it possible to perfectly balance the counterweight and the pistons, ensuring smooth travel always. With permanently closed valves, the air inside the cylinder compresses and decompresses as the pistons move up and down. It provides, therefore, a restoring force. As such, it will store potential energy, just like a spring. ³⁰ See: *The Wavefunction as an Energy Propagation Mechanism*.

³¹ I am grateful to an unknown undergraduate student for posting this solution. Unfortunately, I lost the reference. Whomever recognizes this, please do email as I would like to properly credit the good work.

³² The analogy can be extended to include two *pairs* of springs or pistons, in which case the springs or pistons in each pair would help drive each other.

³³ We did not google references here, but the <u>Wikipedia article on radial engines</u> looks like a good start.

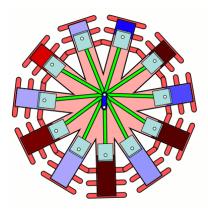


Figure 3: The metaphor of the radial engine (source: Wikipedia)

The point is this: somehow, in this beautiful interplay between linear and circular motion, energy is borrowed from one place and then returns to the other, cycle after cycle. While transferring kinetic energy from one piston to the other, the crankshaft will rotate with a constant angular velocity: linear motion becomes circular motion, and vice versa. Most importantly, we can *add* the total energy of the oscillators to get the total energy of the whole system to get the $E = ma^2\omega^2$ formula. The only thing that remains to be done then, is to substitute for the tangential velocity $v_t = a\omega$. In fact, substituting $a\omega$ for c= $a\omega$ gives us Einstein's mass-energy equivalence relation ($E = mc^2$) is what inspired our mass without mass model of an electron.

Back to the question. Does our metaphor shed any light on the question?

The meaning of the wavefunction

So we have this general idea that the oscillations of the real and imaginary part of the wavefunction, somehow, incorporate the energy conservation law. This interpretation is quite consistent with Feynman's characterization of the wave *equation* as an energy diffusion equation, of course. Let us quote him once more:

"We can think of Schrödinger's equation as describing the diffusion of the probability amplitude from one point to the next. [...] But the imaginary coefficient in front of the derivative makes the behavior completely different from the ordinary diffusion such as you would have for a gas spreading out along a thin tube. Ordinary diffusion gives rise to real exponential solutions, whereas the solutions of Schrödinger's equation are complex waves."³⁴ (Feynman, III-16-1)

So, yes, we get this: the 'complex waves' are just local cyclical things – like circular or elliptical or other regular non-linear waves. Stuff that goes around and around or, when it starts moving linearly, combines linear and circular motion.³⁵ For linear waves – think of sound waves, water waves, radio

³⁴ Feynman further formalizes this in his Lecture on Superconductivity (Feynman, III-21-2), in which he refers to Schrödinger's equation as the "equation for continuity of probabilities". However, the analysis here is really centered on the local conservation of energy, which confirms the interpretation of Schrödinger's equation as an energy diffusion equation.

³⁵ If there is one other paper of ours that we would recommend reading, it is the one that attracts the most attention on ResearchGate – for the right reasons, we think: <u>*De Broglie's Matter-Wave: Concept and Issues*</u>. We

waves or whatever wave that moves from here to there in space – we have real-valued wave equations, but for this circular stuff we have complex-valued wave equations because... Well... Because Euler invented complex numbers and they magically fit the bill when trying to model all of this. So that is clear and obvious enough, but is this interpretation compatible with all of the formalism of quantum mechanics, and with operator theory in particular? It should be: if we know the potential and kinetic energy – *at any point in time* – we should be able to derive position, momentum, and all other relevant physical observables from it, isn't it?

Of course, we admit we should formally show this by reexamining the textbook derivations of operators so as to prove the point. So how can we proceed then? We know we can extract the real and imaginary part using the general $Re(z) = (z+z^*)/2$ and $Im(z) = (z-z^*)/2i$ for a complex-valued number (and, hence, for a function as well) and, hence, we could use this operators and then try to see whether we find anything more interesting than what we already wrote above. Let us quickly do the first step, continuing the electron orbital example. The $\psi(r)$ function is the $\psi_{n,l,m}(\rho, \theta, \Phi)$ function without the complex exponential and is, therefore, the real-valued spatial (time-independent) part of the wavefunction. We, therefore, just get the obvious result that we started out with³⁶:

$$Re[\psi(\mathbf{r},t)] = Re\left[e^{-i(\frac{E}{\hbar}t+\phi)} \cdot \psi(\mathbf{r})\right] = \frac{e^{-i(\frac{E}{\hbar}t+\phi)} \cdot \psi(\mathbf{r}) + e^{i(\frac{E}{\hbar}t+\phi)} \cdot \psi(\mathbf{r})}{2}$$
$$= \frac{e^{-i(\frac{E}{\hbar}t+\phi)} \cdot \psi(\mathbf{r}) + e^{i(\frac{E}{\hbar}t+\phi)}}{2} \cdot \psi(\mathbf{r}) = \cos\left(\frac{E}{\hbar}t+\phi\right) \cdot \psi(\mathbf{r}) = \cos(\omega t+\phi) \cdot \psi(\mathbf{r})$$

$$Im[\psi(\mathbf{r},t)] = Im\left[e^{-i(\frac{E}{\hbar}t+\phi)} \cdot \psi(\mathbf{r})\right] = \frac{e^{-i(\frac{E}{\hbar}t+\phi)} \cdot \psi(\mathbf{r}) - e^{i(\frac{E}{\hbar}t+\phi)} \cdot \psi(\mathbf{r})}{2i}$$
$$= \frac{e^{-i(\frac{E}{\hbar}t+\phi)} \cdot \psi(\mathbf{r}) - e^{i(\frac{E}{\hbar}t+\phi)}}{2i} \cdot \psi(\mathbf{r}) = \sin\left(\frac{E}{\hbar}t+\phi\right) \cdot \psi(\mathbf{r}) = \sin(\omega t+\phi) \cdot \psi(\mathbf{r})$$

This just shows, once again, that the real and imaginary part of our wavefunction (r, t) - yes, we are talking this very complicated functional form which combines power series and derivatives of Legendre polynomials! – varies as a simple sine and cosine *at any point r in space*. A sine and cosine function of what? Time. So what do we have here? It is a clock, once more, but this time it is a clock with a hand whose *length* varies as a function of the position. An elliptical clock, perhaps? What is the formula for an ellipse again?

$$\frac{x^2}{a} + \frac{y^2}{b} = 1$$

That is too simple, obviously! Our x and y here, so to speak, are the $cos(\omega \cdot t + \phi) \cdot \psi(r)$ and $sin(\omega \cdot t + \phi) \cdot \psi(r)$ functions and they are very different beasts! *Real-valued* functions, yes, but complicated

describe the (possible) *geometry* of the matter-wave in full detail there, including a geometric interpretation of the de Broglie wavelength.

³⁶ We took the $e^{im\Phi}$ factor out of the and replaced the m· Φ term by an arbitrary phase shift φ .

functions: just look at those polar graphs once more, or the wonderful shapes of those subshells in 3D illustrations!³⁷ However, the functional form for an ellipse usefully reminds of what a function actually is: a constraint on a set of variables. So what constraints do we have here?

Well... The wavefunction is a solution for a definite energy state, right? Hence, we should get the energy out the wavefunction and then we get an equation $E = E_n$ with $\psi(r)$ in it, and then... Well... Then what? We should just apply our energy operator $H = -\frac{\hbar^2}{2m}\nabla^2 + V(r)$, right? And we should just get Schrödinger's wave equation again – which we started out with, right? Let us check, though, just to make sure we are not finding anything new or doing something wrong here. In fact, let us recap where those formulas for the energy operator come from, so we know what is what – not approximately, but *exactly*? These operators are actually used to calculate *average* or *expected* values³⁸. So we are not assuming anything about the value for the energy, and we just take the value for the *average* energy of the system. This means we are going to start off by *not* assuming that the system (read: the state of our electron in its orbital – whatever that may be) should be in a *definite* energy state. The formula³⁹ is an integral, taken over the whole volume of the atom:

$$\langle \mathbf{E} \rangle_{average} = \int \langle \psi | \mathbf{H} | \psi \rangle \, d\text{Vol} = \int \psi^* \mathbf{H} \psi \, d\text{Vol} = \int \mathbf{H} \psi^* \psi \, d\text{Vol} = \int \mathbf{H} | \psi |^2 d\text{Vol}$$

$$\text{with:} \quad \mathbf{H} = -\frac{\hbar^2}{2m} \nabla^2 + V(\mathbf{r})$$

Are we allowed to write that Hamiltonian in front of the H expression? Good question. It is, but you should double-check: note that ψ is, once again, the $\psi(\mathbf{r})$ function only: it does *not* include the time-dependent part. How should we think of this? You will want to think we have averaged the energy over a *cycle* of the oscillation. Sorry for mixing high-class math with simple illustrations once again, but inserting an easy reminder of how potential and kinetic energy vary and add up over a full cycle of an oscillation might help here (Figure 4).

 $^{^{37}}$ That is the reason why we keep putting the ϕ factor in: it is just a phase shift, but we need the quantum number m also for our derivatives (as an order number) of the Legendre polynomials: we can neatly separate out the time-dependent part but – for the time being, at least – we cannot simply forget about it!

³⁸ We use both as synonyms. To be precise, the expected value is the *average* value which a variable will take when an experiment (so that is a *measurement*) is repeated a large or (theoretically) an infinite number of times even, and so the mean (or weighted average) of all the values is calculated along the way.

³⁹ In case the reader would like to check the formulas we are using (or our consistency in terms of definitions), we refer to Feynman's treatment of operators and more in particular, <u>Feynman's Lectures, section III-20-3</u> (average energy of an atom).

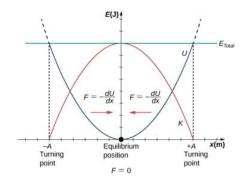


Figure 4: Kinetic (K) and potential energy (U) of an oscillator⁴⁰

So what do we have here? The absolute square of the wavefunction is the probability of finding our electron at \mathbf{x} , so when integrating $|\psi(\mathbf{r})|^2$ over the volume, we get 1, right? All probabilities add up to 1: $\int |\psi(\mathbf{r})|^2 d$ Vol = 1. Yes. For normalized wavefunctions. If we do *not* normalize our wavefunction, we should use this formula for the energy:

$$\langle \mathbf{E} \rangle_{average} = \frac{\int \psi^* \mathbf{H} \psi \, d \mathbf{Vol}}{\int \psi^* \psi \, d \mathbf{Vol}}$$

But what are we talking about here? How would we go about normalizing, anyway? The $\int |\psi(\mathbf{r})|^2 d$ Vol = 1 condition amounts to:

$$\int \psi^* \psi \, d\text{Vol} = 1 \iff \frac{\int \psi^* H \psi \, d\text{Vol}}{\langle E \rangle_{average}} = 1 \iff \int \psi^* H \psi \, d\text{Vol} = \int H |\psi|^2 d\text{Vol} = \langle E \rangle_{average}$$

And what is all that talk about averaging energy if we are talking *definite* energy states and we know we are averaging energy *over a full cycle of the oscillation*? Because that is what we are doing when separating out the time-dependent part of the wavefunction, right? Right. So we can just write this:

$$E = \int H|\psi|^2 dVol = \int H|\psi|^2 dVol = \int -\frac{\hbar^2}{2m} \nabla^2 |\psi|^2 + V(r)|\psi|^2 dVol = \int T|\psi|^2 + V|\psi|^2 dVol$$

So what are we doing here? We are applying our energy operators – total energy (H), kinetic energy (T) and potential energy $(V)^{41}$ – to the probability $P(x) = |\psi(x)|^2$. But the energy of what? It must be the energy of our pointlike electron if and when it would happen to be at x, right? And then we multiply that value with the *probability* of the electron being there. So what we are doing is this: we do sum all of the energy *densities* – a sum of an infinite number of infinitesimally small volume elements (I am just reminding you of the definition of a 3D integral) – and, no surprise, we get the total energy E which – in turn – is used to *normalize* the probabilities that we are using. We can illustrate this *physical* normalization condition by writing:

⁴⁰ You will find this diagram in many texts, but we took this one from the <u>https://phys.libretexts.org/</u> site—excellent hub for open-access textbooks.

⁴¹ We apologize once again for not using fancier hat or script notation. We think it is not necessary: the meaning of the symbols is clear from the context.

$$\int \psi^* \psi \, d\text{Vol} = 1 \Leftrightarrow \int \text{H} |\psi|^2 d\text{Vol} = \int \text{H} P(\boldsymbol{r}) \, d\text{Vol} = \text{E}$$

Is this a circular argument? It is, but we think it is a useful one (in the sense that it helps us understanding what is what here⁴²).

So where are we now? We now understand how potential and kinetic energy slosh back and forth in this system, always adding up to some constant, but we forgot about the original question: the real and imaginary parts of the wavefunction. We abstracted away from that by looking at the spatial part of the wavefunction only. So let us look at the whole thing by plugging the time-dependence back in. So we have a wavefunction which we can not only split into a time bit and a space bit – a simple scalar product of both, to be precise:

$$\psi(\mathbf{r}, t) = \psi(\mathbf{r}) \cdot e^{-i \cdot [(E/\hbar) \cdot t + \phi]}$$

Now, the time-dependent thing is the simplest of complex exponentials and allow us to also nicely separate everything out into a real and an imaginary bit:

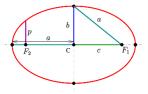
$$Re[\psi(\mathbf{r},t)] = \cos(\omega t + \varphi) \cdot \psi(\mathbf{r})$$
$$Im[\psi(\mathbf{r},t)] = \sin(\omega t + \varphi) \cdot \psi(\mathbf{r})$$

These are two orthogonal vectors in the complex plane⁴³ and we can, therefore, apply Pythagoras's Theorem:

$$[\cos(\omega t + \varphi) \cdot \psi(r)]^2 + [\sin \cdot \psi(r)]^2 = [\cos^2(\omega t + \varphi) + \sin^2(\omega t + \varphi)]\psi^2(r) = \psi^2(r) = |\psi(r)|^2$$

However, this just reminds us of the fact that the square of the modulus of a real number (the *absolute* square) is just the squared number itself. And taking the square root back allows for positive or negative (but always real-valued) amplitudes (spatial bit only), of course. But this does not add anything to our interpretation of the wavefunction. Can we add anything to the interpretation by trying to find some latus rectum formula? It might be possible, but we do not think so.⁴⁴

⁴⁴ The latus rectum formula is $a \cdot p = b^2$, with a, p and b the lengths as depicted below.



The latus rectum formula popped up quite naturally in <u>our geometric interpretation of the *de Broglie* wavelength, which was quite surprising and very interesting. However, our earlier <u>attempt to interpret Schrödinger's orbitals in</u> <u>terms of elliptical orbitals</u> failed. We, therefore, regret this early paper remains popular, even if it gave us early ideas on the nature of Schrödinger's wave *equation* (not wavefunction) as an energy diffusion equation.</u>

⁴² We hope it helps the understanding of the *nature* of the wavefunction for the reader too, but that is for him or her to judge, of course.

⁴³ A complex *space* is usually associated with complex-valued coordinates or may have some other meaning. The complex *plane* is just two-dimensional Cartesian space, with the *x*-axis representing the real part (the axis with the cosine values) and the *y*-axis representing the imaginary part (the axis with the sine values).

So that is it, then:

- 1. Kinetic and potential energy sloshing back and forth and, obviously, adding up to the total energy; and
- 2. The sum of squares of the real and imaginary part adding up to give us an *energy density* (non-normalized wavefunction) or a (normalized) *probability* $P(\mathbf{r}) = |\psi(\mathbf{r})|^2$ to find the electron as a function of the position vector \mathbf{r} .

We think we found an awful lot of *meaning* but, yes, do we really *get* it? Maybe. Maybe not. Can we do better? Frankly, we feel we may not be able to do any more explaining that what we have done already here. The bottom line may well be this: the real and imaginary part of the wavefunction(s) – i.e. the solution(s) to the wave equation that applies to the situation at hand – combines not only the energy conservation law (potential and kinetic adding up to the (constant) total) but all of physics, plus Pythagoras's (complex number theory, that is), operator theory and... Well... All of the math in-between.

Hence, it actually does like some kind of miracle that, somehow, all laws of physics – and all of geometry, of course! – combine into Euler's function. So that it is then, and there is no further explanation: we should marvel at the fact that we sort of get this. So that is all of the mystery of quantum mechanics, then. And we should conclude that Leonhard Euler truly was the Master of Masters.⁴⁵

Jean Louis Van Belle, 24 October 2020

⁴⁵ I am just quoting one of the other great polymaths of history here, Pierre-Simon Laplace, who is said to have said: "Read Euler, read Euler, he is the master of us all!"

Annex: Spin and the imaginary unit

When thinking of spin as *physical* angular momentum, one can easily integrate the concept of spin in the elementary wavefunction by thinking about the *direction* of motion, as illustrated below (**Figure 5**): we can go from the +1 to the -1 position on the unit circle taking opposite directions.

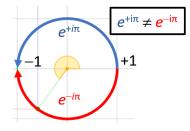


Figure 5: $e^{+i\pi} \neq e^{-i\pi}$

Hence, combining the + and – sign for the imaginary unit with the direction of travel, we get four mutually exclusive structures for our electron wavefunction (see Table 1).

Spin and direction of travel	Spin up (<i>J</i> = +ħ/2)	Spin down (J = -ħ/2)
Positive <i>x</i> -direction	$\psi = \exp[i(kx-\omega t)]$	$\psi^* = \exp[-i(kx-\omega t)] = \exp[i(\omega t-kx)]$
Negative <i>x</i> -direction	$\chi = \exp[-i(kx+\omega t)] = \exp[i(\omega t-kx)]$	$\chi^* = \exp[i(kx+\omega t)]$

Table 1: Occam's Razor: mathematical possibilities versus physical realities

Unfortunately, the mainstream interpretation of quantum mechanics does not integrate the concept of particle spin from the outset because the + or – sign in front of the imaginary unit (*i*) in the elementary wavefunction ($a \cdot e^{-i \cdot \theta}$ or $a \cdot e^{+i \cdot \theta}$) is thought as *a mathematical convention* only. This non-used *degree of freedom* in the mathematical description then leads to the *false* argument that the wavefunction of spin-½ particles has a 720-degree symmetry. Indeed, physicists treat –1 as a *common phase factor* in the argument of the wavefunction.⁴⁶ However, we should think of –1 as a complex number itself: the phase factor may be $+\pi$ or, alternatively, $-\pi$: when going from +1 to –1 (or vice versa), it matters how you get there—as illustrated above.⁴⁷

⁴⁶ Mainstream physicists therefore think one can just multiply a set of amplitudes – let us say *two* amplitudes, to focus our mind (think of a beam splitter or alternative paths here) – with –1 and get the same *physical states*. ⁴⁷ The quantum-mechanical argument is technical, and so I am not going to reproduce it here. I do encourage the reader to glance through it, though. See: *Euler's Wavefunction: The Double Life of – 1*. Note that the $e^{+i\pi} \neq e^{-i\pi}$ expression may look like *horror* to a mathematician! However, if he or she has a bit of a sense for geometry and the difference between identity and equivalence relations, there should be no surprise. If you are an amateur physicist, you should be excited: it is, effectively, the secret key to unlocking the so-called mystery of quantum mechanics. Remember Aquinas' warning: *quia parvus error in principio magnus est in fine*. A small error in the beginning can lead to great errors in the conclusions, and we think of this as a rather serious error in the beginning!