

The Electron in a Potential

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1. Stopwatch rotation for an electron in a potential

For a photon we found that the hand of the quantum stopwatch rotates with frequency f given by the equation:

$$f = \frac{E}{h} \quad (\text{for the photon -- zero mass}) \quad (1)$$

This is the frequency with which the stopwatch hand rotates (rotations/second) as the photon explores alternative paths.

For the free electron (the electron free of any forces or potentials) we postulated that the hand of the quantum clock rotates at the following rate:

$$f = \frac{KE}{h} \quad (\text{for the free electron}) \quad (2)$$

Here KE is the kinetic energy of the electron. Now suppose the electron has potential energy, possibly due to the electric attraction of a positively-charge nucleus. How do we combine kinetic and potential energy to find a frequency for the stopwatch rotation when an electron explores a path in this potential? We are tempted to use equation (2) also for this case, with kinetic energy KE replaced by total energy E equal to kinetic energy plus potential energy: $E = KE + PE$.

WRONG!

Why wrong? Because if we should take $f = E/h$ for the electron, substituting the total energy in this formula, the minimum number of rotations would favor paths in which PE , the potential energy, is low to make $E = KE + PE$ low and hence rotation rate f low. Between baseball pitcher and catcher (playing in a vacuum!), the thrown electron would drop in height (lowering its PE and slowing its quantum clock) and then rise up again to keep its fixed appointment with the catcher's mitt. By going *down* and then rising, the pitched electron decreases its PE and minimizes the number of rotations of its quantum clock between pitcher and catcher. But this is absurd. Antigravity? Impossible! With this WRONG choice for frequency, quantum physics would not go over smoothly into classical mechanics as the mass of the thrown particle increases from that of an electron to that of a baseball. So it is WRONG to use the SUM of KE and PE in calculating the rate of rotation of the stopwatch as the electron explores paths.

But we *know* how a baseball flies. We *know* the quantity that is minimized in the classical path. The baseball moves so as to minimize the ACTION between fixed events of pitching and catching—as described in the Feynman lecture on the Principle of Least Action, Lecture 19 of Volume II of *The Feynman Lectures in Physics*. and in the earlier section of this manual titled “The Principle of Least Action.” ALMOST ALL of the classical mechanics for a single particle can be derived from the Principle of Least Action. And this principle involves summing up over time the contributions from the expression $KE - PE$, with a MINUS sign before the potential energy PE .

The quantum result, it turns out, simply adapts the thing that we sum over time to get the classical action, namely $KE - PE$.

The rate of rotation (in cycles/second) of the stopwatch hand for an electron exploring a path (for speeds much less than the speed of light) is:

$$f = \frac{KE - PE}{h} \quad \text{(for the electron)} \quad (3)$$

We find the number of rotations along a worldline by a summing process: During a small increment of time dt , the number of rotations (or fraction of a rotation) is $f dt = (KE - PE) dt/h$. We sum this for all time increments along the worldline:

$$\left(\begin{array}{c} \text{rotations} \\ \text{along a} \\ \text{worldline} \end{array} \right) = \frac{\int_{\text{along worldline}} (KE - PE) dt}{h} \quad (4)$$

But the numerator on the right side of (4) is simply the action S (defined in equation (1) in the preceding section on the Principle of Least Action). Hence the number of rotations along a worldline is just:

$$\left(\begin{array}{c} \text{rotations} \\ \text{along a} \\ \text{worldline} \end{array} \right) = \frac{\left(\begin{array}{c} \text{Action} \\ \text{along that} \\ \text{worldline} \end{array} \right)}{h} = \frac{S}{h} \quad \text{(for the electron)} \quad (5)$$

Looking at equations (4) and (5), we see that the number of revolutions between pitcher and catcher can be made minimum by *increasing* PE in order to reduce the frequency f of the quantum clock—since PE enters these equations with a minus sign. Increase PE by letting the path rise. But it cannot rise too far, because then KE must increase so that the electron can rush along the longer path to keep the fixed appointment with the catcher’s mitt. [Both events “pitch” (emit) and “catch” (detect) are fixed in quantum as well as in classical descriptions.] The actual path is a

compromise between increasing PE (that lowers the frequency f) and increasing KE (that raises f). In a vacuum, then, the greatest contribution to the resulting arrow for detection of the electron comes from trajectories near the classical path of parabolic motion in a uniform vertical gravitational field. With increasing mass, the path of minimum quantum rotations for the electron goes over smoothly to the path of minimum classical action for the baseball. *We have found a crucial connection between classical mechanics and quantum mechanics.*

Actually, we have found something vastly more important: *We have found the quantum mechanical basis for most of classical mechanics.* Classical mechanics has no answer to the question, “WHY does a particle moving in a potential (including zero potential) follow the path predicted by the Principle of Least Action?” The answer—true for both quantum and classical worlds—is, “Because this path minimizes the number of rotations of the quantum clock.”

So what is the DIFFERENCE between the quantum world and the classical world? The answer is embodied in Planck’s constant h in the *denominator* of the right-hand sides of equations (3) thru (5)—along with the mass m of the particle hidden in the *numerator*. The electron has the smallest mass of any stable particle that we know. A small mass in the numerator in (3) “balances” the tiny value of h in the denominator. The resulting frequency f (dividing numerator by denominator) can be low enough so that total clock rotations along nearby paths are not too different. A slightly different path can have a total rotation of, say, one-eighth turn more than the path for minimum total rotation. Then to calculate the resulting arrow, you must take account of this nearby path, along with others. The electron “sniffs out” a “fuzzy” range of paths around the minimum-total-rotation path; this is what we *mean* by quantum behavior!

In contrast, for a large mass in the numerators in equations (3) thru (5)—the mass of a baseball, for example—the tiny value of h in the denominator makes the frequency f *extremely* rapid. In this case, a slightly different path will have a total rotation hundreds of turns more than the path for minimum total rotation. In this case contributions from all nearby paths tend to cancel out. In the limit of large mass, only the single path of minimum rotation needs to be taken into account, the path predicted by the Principle of Least Action. The baseball appears to follow a single path; that is what we *mean* by classical behavior!

The electron can also explore all paths inside an atom or molecule. In this case the nuclear charge provides potential energy that influences the rotation rate of the electron clock—different rotation rates for different distances from the nucleus. This rotation rate changes as the electron explores regions of different potential PE

along each path. This simple story is complicated by spin and by the presence of other electrons in the atom or molecule. You didn't *really* think that we would also cover all of chemistry, did you?

3. **This Is a Derivation?**

The above story line is NOT a derivation. There *is* no known derivation of the fundamental laws of quantum mechanics. Certainly no derivation can come from classical physics!

No fundamental derivation appears possible. Nevertheless, there is powerful evidence for the correctness of the derivation. Long ago Feynman¹ showed that this “stopwatch” way of thinking leads rigorously to the usual machinery of quantum physics—expressed in the so-called Schroedinger equation. And the Schroedinger equation is the basis for our predictions about all non-relativistic quantum structures and experiments, including chemical bonding and the periodic table.

Notice two *limitations* of the classical Principle of Least Action that turn out to be *advantages* when this principle is applied to quantum mechanics:

FIRST, the Principle of Least Action requires that we fix in both space time the two events of “pitch” and “catch.” But this is an advantage in quantum mechanics, where we want to choose the event of “emission” and also choose the time and place where we will try to “detect” the particle. So the Principle of Least Action limits the description of motion to just those conditions we want for our quantum description.

SECOND, the Principle of Least Action does not apply classically when there is friction. You must be able to define a potential, which you cannot do if friction is all the time robbing your moving stone of energy. But this is OK in quantum mechanics, because there *is no* friction at the atomic level: potential plus kinetic energy is conserved rigorously in non-relativistic quantum physics. Once again, the Principle of Least Action limits attention to just those conditions we want for our quantum description.

4. **Terminology**

The function $KE - PE$ for a low-velocity particle is called the *Lagrangian* and given the symbol L (sometimes a script L). So we have:

$$L = KE - PE \tag{6}$$

and from equation (3):

$$f = \frac{KE - PE}{h} = \frac{L}{h} \quad (\text{electrons \& other particles with mass}) \quad (7)$$

Those who would like to measure clock rotation rate ω in radians per second instead of f in revolutions per second can use the usual relation between the two:

$$\omega \equiv 2\pi f = 2\pi \frac{L}{h} = \frac{L}{\hbar/2\pi} = \frac{L}{\hbar} \quad (\text{electrons, etc.}) \quad (8)$$

Here \hbar , written as h with a little diagonal strike across it, is pronounced “h-bar” and stands for the expression:

$$\hbar \equiv \frac{h}{2\pi} \quad (9)$$

So now we know how fast the quantum clock rotates for the electron.

Appendix: Some Formalism Leading Toward the Wave Function

We try to avoid formalism. If mathematics irritates and frustrates you, skip the following. But some people like the clean condensation that mathematics can bring. And a big payoff in this case is an understanding of the quantum mechanical **wave function**.

Feynman develops a set of rules for reckoning the final arrow at a detector. The probability that the detector will record the particle is proportional to the square of the length of this final arrow. The rules can be placed in a hierarchy derived from pages 37 and 61 of *QED*:

GRAND PRINCIPLE: The probability of an event is proportional to the square of the length of a “resulting arrow,” this arrow called the “quantum amplitude.” (Feynman calls it by the confusing name “probability amplitude.”)

RULE FOR ALTERNATIVE PATHS: If an event can happen in alternative ways, draw an arrow for each way, then combine (“add”) the arrows by hooking the head of one to the tail of the next. The final arrow is then drawn from the tail of the first arrow to the head of the last arrow. This final arrow is the resulting arrow used in the GRAND PRINCIPLE

RULE FOR SEQUENTIAL STEPS IN EACH PATH: When each way that an event can happen involves a series of steps in sequence, think of each step as a *shrink* and *turn* of the little arrow. To find the arrow for that complete path, multiply the shrinks for all steps in the path and add the angle changes (turns) for all steps in the path. The arrow

for that complete path is added to others from ALTERNATIVE PATHS to give the resulting arrow used in the GRAND PRINCIPLE.

Is there a mathematical quantity that behaves in these ways? First, one must be able to ADD such quantities as arrows are added. Second, MULTIPLICATION of such quantities must mean finding the product of their magnitudes and the sum of their angles of rotation.

Such a mathematical quantity is the complex number, which can be expressed in two forms that are entirely equivalent:

$$Ae^{i\theta} \equiv A \cos \theta + iA \sin \theta \quad (10)$$

Here $e = 2.71828 \dots$ is the base of **natural logarithms** and $i \equiv \sqrt{-1}$ is the basis of **imaginary numbers**. **Complex numbers** combine real and imaginary numbers.

REFERENCE: *The Feynman Lectures on Physics*, Volume I, Chapter 22, especially pages 22-7 thru 22-10.

Adding two complex numbers means adding their real parts and then separately adding their imaginary parts. This is equivalent to adding separately the x -components and the y -components of two arrows to obtain the components of the resulting arrow. For two complex numbers, designated by the subscripts 1 and 2, we have:

$$\begin{aligned} Ae^{i\theta} &\equiv A_1e^{i\theta_1} + A_2e^{i\theta_2} \\ &= A_1 \cos \theta_1 + iA_1 \sin \theta_1 + A_2 \cos \theta_2 + iA_2 \sin \theta_2 \\ &= (A_1 \cos \theta_1 + A_2 \cos \theta_2) + i(A_1 \sin \theta_1 + A_2 \sin \theta_2) \end{aligned} \quad (11)$$

Multiplying complex numbers is even easier:

$$Ae^{i\theta} \equiv A_1e^{i\theta_1} \times A_2e^{i\theta_2} = (A_1 \times A_2)e^{i(\theta_1+\theta_2)} \quad (12)$$

This is a direct example of the rule for finding the arrow for a sequence of steps in one path: MULTIPLY the magnitudes of the arrows for each sequential step in the path and ADD the angle changes. If A_2 is less than unity, multiplying A_1 by A_2 corresponds to a “shrink.” Adding the angles corresponds to a “turn.”

The probability for the final outcome is proportional to the square of the magnitude (the square of the “length” or A -value) of the resulting complex number.

You may have been told that quantum mechanical quantities, such as wave functions, are *complex* functions. Why is this so? Complex numbers and complex functions are just ways we combine the little arrows to form a resulting arrow, the

probability amplitude, whose square is proportional to the probability. Complex numbers are used to track the shrinking, turning, and adding of those little arrows that lead to a resulting arrow and a final probability.

Using this notation, we can describe the motion of the electron along alternative paths. The angles θ used in the complex notation are expressed in radians. The rotation rate ω for the electron clock in radians per second is given by combining equations (6) and (8).

$$\omega = \frac{L}{\hbar} = \frac{KE - PE}{\hbar} \quad (13)$$

How many times will the little clock hand rotate along a given path (call it path k) from initial event 1 to final event 2? We can compute this, starting with the action S for that path:

$$S_k = \int_{\text{path } k} (KE - PE) dt \quad (14)$$

Here each path is required to start at the same initial event 1 and to end at the same final event 2, so the time along the path is the same for every alternative path. This means that the kinetic energy is different for different paths, and *total energy is not the same for alternative paths*. (For an arbitrary path, the total energy may not even be constant along this single path.) But for large-mass particles the little arrows from all paths point in very different directions and tend to cancel out except those near the path of least action, for which the little arrows point in nearly the same direction. For these paths the total energy is conserved, as we saw in the ACTION software.

The contribution to the probability amplitude for a single path is given by:

$$A_k e^{iS_k/\hbar} \quad (15a)$$

For those of us with failing eyesight, these exponentials may be too small, so we use the function $\exp()$ to represent the exponential with e :

$$A_k \exp(iS_k/\hbar) \quad (15b)$$

Then the probability amplitude for the given outcome is reckoned from the sum of these contributions for every alternative path (indexed by k) between a fixed initial event 1 and a fixed final event 2:

$$\text{Probability amplitude (from 1 to 2)} = \sum_{\substack{\text{all paths } k \\ \text{from event 1}}} A_k e^{iS_k/\hbar} \quad (16a)$$

or

$$\text{Probability amplitude (from 1 to 2)} = \sum_{\substack{\text{all paths } k \\ \text{from event 1}}} A_k \exp(iS_k / \hbar) \quad (16b)$$

This is the probability amplitude that the electron starts at a particular initial event 1 and arrives at a particular final event 2 placed at, say, x and t . We can call this the **wave function** $\psi(x,t)$ for a particle emitted from event 1:

$$\psi(x,t) = \sum_{\substack{\text{all paths } k \\ \text{from event 1}}} A_k e^{iS_k/\hbar} \quad (17a)$$

or

$$\psi(x,t) = \sum_{\substack{\text{all paths } k \\ \text{from event 1}}} A_k \exp(iS_k / \hbar) \quad (17b)$$

This is the meaning of Feynman's statement in his abstract for the 1948 article in *Reviews of Modern Physics*:¹

“The total contribution from all paths reaching x,t from the past is the wave function $\psi(x,t)$.”

Reference

¹R. P. Feynman, “Space-Time Approach to Non-Relativistic Quantum Mechanics,” *Reviews of Modern Physics*, Volume 20, Number 2, April 1948, pages 367 - 387.