

“Zur quantendynamik des Electrons,” Sitzber. preuss. Akad. Wiss, Phys.-Math. Klasse **3** (1931), 63-72;
Ges. Abh., v. III, pp. 369-379.

On the quantum dynamics of the electron

By

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§ 1. The best (indeed, the *only*) tool that we currently possess for describing the dynamics of electrons when one includes spin and relativistic effects is the DIRAC wave equation. In the field-free case, it reads:

$$\kappa \frac{\partial \psi}{\partial t} + H\psi = 0, \quad (1)$$

with

$$\kappa = \frac{h}{2\pi i}, \quad H = c (\alpha_1 p_1 + \alpha_2 p_2 + \alpha_3 p_3 + \alpha_4 mc).$$

The operator H then corresponds to the “kinetic” energy of the electron (classical analogue: $mc^2 / \sqrt{1-\beta^2}$). One understands the p_k to mean the operators $\kappa \frac{\partial}{\partial x_k}$, and the

α_k to mean certain linear transformations of $\psi_1, \psi_2, \psi_3, \psi_4$ with numerical coefficients. It is convenient to regard the *index* of ψ as a further argument (viz., the “spin coordinate” ζ) upon which ψ depends, in addition to x_1, x_2, x_3, t . Namely, one will then have the same right to drop it from the notation, as one did above, as one has for the remaining four arguments.

DIRAC was the first to point out the following grave inconvenience that separated his electron dynamics from all of the previous ones, to the extent that they satisfied the relativity constraint: *The H-operator above also has negative eigenvalues.*

One solves the eigenvalue problem:

$$H\psi = E \cdot \psi \quad (2)$$

by the Ansatz:

$$\psi = u(\zeta) \cdot e^{\frac{1}{\kappa}(p'_1 x_1 + p'_2 x_2 + p'_3 x_3)} \quad (3)$$

(E, p'_1, p'_2, p'_3 are ordinary numbers, namely, the eigenvalues of energy and the impulse components; $u(\zeta)$ is a function of only the spin index – i.e., a quadruple of coefficients).

It then turns out that E is not determined uniquely by p'_1, p'_2, p'_3 . The function $u(\zeta)$ indeed admits the determination that yields:

$$E = +\sqrt{c^2(p_1'^2 + p_2'^2 + p_3'^2) + m^2c^4}, \quad (4)$$

but also one for which E will be equal to the negative square root. ψ will then be an eigenfunction of negative kinetic energy. Obviously, one cannot ignore that class of eigenfunctions. One must necessarily develop them in an *arbitrary* initial state in eigenfunctions of H just like the other ones, when that is true. Without those “negative” functions, the system of eigenfunctions would not be complete.

At any rate, all of that would be thoroughly irrelevant if one were treating the *force-free* case. Then, if an aggregate of “positive” eigenfunctions were present at some time point then that state of affairs would be preserved for all time points as a result of equation (1). One could justly contradict that by saying that the basic equation also admits other solutions that are not, however, realized in nature.

Things behave differently in a force field. In order to avoid misunderstanding, I shall establish the following terminology: A function of x_1, x_2, x_3, ζ is called *positive* when the only eigenfunctions enter into their development in terms of eigenfunctions of the *force-free* (!) operator H are ones that belong to positive eigenvalues of H . By contrast, if the only eigenfunctions that enter into the development belong to negative eigenvalues then the function of x_1, x_2, x_3, ζ in question shall be called *negative*. Since there is no value $E = 0$, and furthermore, one always has:

$$|E| \geq mc^2, \quad (5)$$

one will immediately see the validity of the following two theorems:

1. Any function of x_1, x_2, x_3, ζ can be decomposed uniquely into a positive and a negative part.
2. Any positive function is orthogonal to any negative function.

We now consider the case of a force field – for example, a central COULOMB force.

The potential energy $\left(-\frac{e^2}{r}\right)$ will then get added to H . In place of equation (1), one will find:

$$\kappa \frac{\partial \psi}{\partial t} + K\psi = 0,$$

with:

$$K = H - \frac{e^2}{r}. \quad (6)$$

It will then emerge that this equation will no longer have the property that a positive ψ -function needs to stay positive. Quite the contrary, from (6), a positive initial-value function will already be mixed with a negative component in the next moment. The

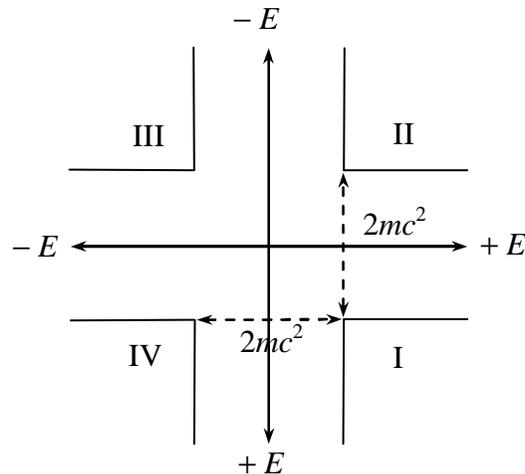
eigenfunctions of K are no longer purely positive either, but they will have negative additions, which are admittedly very small. With the usual interpretation, for a hydrogen atom in the stationary state, there would then exist a certain (if only very slight) probability that its electron would possess a negative kinetic energy (classical analogue: $mc^2 / \sqrt{1-\beta^2}$) that is smaller than $-mc^2$. The validity of these (otherwise generally known) assertions will become clearer in what follows in a very simple way.

The goal of this note is to alter DIRAC's theory in such a way that the complications will be avoided. Equation (1) will be the basis for everything. However, the potential will be introduced into the equation in a somewhat different way, and indeed in such a way that, for example, the hydrogen eigenfunctions prove to be purely positive, and that a positive function will always remain positive, even in an arbitrary force field. That shows that the agreement with experiments will be preserved at the following important points:

1. The fine structure of hydrogen and He^+ lines.
2. The linear and quadratic Stark effect.
3. The linear Zeeman effect of hydrogen and He^+ lines.

It will be tested at many other points, but the present analysis will give some confidence in the attempt that will now be discussed.

§ 2. A dominant role is played in that analysis by the concept of *even* and *odd* operators. An operator shall be called *even* when it takes every positive function (cf., the definition in § 1!) to another positive one and any negative function to another negative one. An operator will be called *odd* when it makes every positive function negative and every negative positive. If we consider an arbitrary operator in a matrix schema in which the force-free Hamiltonian operator is diagonal (cf., the figure). Rows and columns are indexed by the eigenvalue E , which runs from $-\infty$ to $-mc^2$ and then again from $+mc^2$ to $+\infty$. The locations that are inside of a central cross with the beam width $2mc^2$ will then be meaningless, and the matrix field will decompose into four completely separate sub-regions I, II, III, IV. An *even* operator is obviously one that has non-vanishing matrix elements merely in the regions I and III, while an *odd* one is restricted to II and IV.



Any operator can be decomposed uniquely into an even and an odd part ([†]):

$$A = G + U.$$

If A is Hermitian then G and U will be, as well. If neither G nor U is identically zero then we will call A “mixed,” and otherwise “pure.” (When one says that an operator is “pure,” that means that it is either even or odd.) Similarly, we would like to call a *function* of x, y, z, ζ *pure* when it is either positive or negative, and *mixed* when it contains components of both kinds.

A product of several pure operators will be pure, and indeed even or odd, according to whether the number of odd operators is even or odd, respectively.

The *expectation value* of an odd operator U is zero for a pure wave function ψ (since $U\psi$ has the opposite “sign” to ψ , and is then orthogonal to it).

The complication that was mentioned in § 1 can now be formulated very simply. Whereas the field-free operator H is obviously even, it will obviously cease to be precisely even when potentials appear. For example, K in equation (6) will no longer be even. $1/r$ contains an odd part that we would now like to determine, even if it is very small. If one writes the wave equation (6) in the form:

$$\kappa d\psi = -K\psi \cdot dt$$

then it will be clear that, even if a wave function is positive at one time-point, it will be mixed with negative components at a subsequent time point. Obviously, a mixed operator can have a pure eigenfunction only in entirely exceptional cases, since it is *simultaneously* an eigenfunction of its even and odd parts, and indeed with an eigenvalue of zero for the latter. It will then follow from:

$$A \chi_+ = (G + U) \chi_+ = A' \cdot \chi_+$$

upon splitting into even and odd parts that:

$$G\chi_+ = A \chi_+ \quad \text{and} \quad U\chi_+ = 0.$$

The same thing will be true for χ_- (¹). An odd operator also has mixed eigenfunctions, in general, and a pure one can possess at most the eigenvalue zero.

An even operator G can always be given a pure system of eigenfunctions. If it possess a mixed eigenfunction:

$$G(\chi_+ + \chi_-) = G' \cdot (\chi_+ + \chi_-)$$

then it will follow upon splitting that:

$$G\chi_+ = G' \cdot \chi_+ \quad \text{and} \quad G\chi_- = G' \cdot \chi_- ;$$

([†]) Translators note: $G = \textit{gerade} = \text{even}$, $U = \textit{ungerade} = \text{odd}$.

(¹) The index + or – on a function shall always express the idea that it is composed of purely-positive or purely-negative parts.

i.e., χ_+ and χ_- are each eigenfunctions with *the same* eigenvalue G' .

§ 3. We now have to split the operator of the COULOMB field $1/r$ into even and odd parts, but then some other operators, as well. The following simple criterion proves to be useful: I call $C_1 = HA - AH$ the *commutator* of A with H . I then refer to the commutator of C_1 with H , and therefore, $HC_1 - C_1H = C_2$, as the *second* commutator of A with H . The *third* commutator is $HC_2 - C_2H$, etc. Likewise, I call $HA + AH$ the *first anticommutator*, its anticommutator with H , the *second anticommutator* of A with H , etc. One easily convinces oneself:

If the first or any *finite* commutator of A with H vanishes identically then A will be even. By contrast, A is odd when the first or any finite anticommutator with H vanishes. Here is the proof: If one imagines the equation that expresses the assumption as being written in the matrix schema of H then its $(k, l)^{\text{th}}$ matrix element will read:

$$A_{kl}(E_k \mp E_l)^n = 0.$$

The upper sign is true for the commutator, and the lower one for the anticommutator, and it is assumed that the n^{th} one will vanish. In the former case, one will have the vanishing of all A_{kl} in the regions II and IV of the figure, since $|E_k - E_l| \geq 2mc^2$ there, and in the latter case, the A_{kl} will vanish in I and III, since $|E_k + E_l| \geq 2mc^2$ there.

We next decompose one of the DIRAC matrices α_k ($k = 1, 2, 3$). The known commutation relations:

$$\alpha_i \alpha_k + \alpha_k \alpha_i = 2 \delta_{ik}$$

easily imply that:

$$H \alpha_k + \alpha_k H = 2 c p_k,$$

or, when written otherwise:

$$H (\alpha_k - c H^{-1} p_k) + (\alpha_k - c H^{-1} p_k) H = 0.$$

Hence:

$$\eta_k = \alpha_k - c H^{-1} p_k \quad (7)$$

is odd, and one will have the decomposition:

$$\alpha_k = c H^{-1} p_k + \eta_k. \quad (8)$$

The first summand on the right then commutes with H , and is thus even. As was explained in a previous place ⁽¹⁾, it represents the “macroscopic” velocity of the electron (as a fraction of the speed of light), while α_k is the “true” velocity $\left(\frac{1}{c} \frac{dx_k}{dt}\right)$ in DIRAC’s theory. For measurable electron velocities, the even parts of α_k are then relatively negligible, so the α_k are odd, “for the most part” (i.e., for $k = 1, 2, 3$).

That will then imply the following decomposition for a Cartesian coordinate:

⁽¹⁾ These Sitzungsberichte, 17 June 1930; pp. 422.

$$\left. \begin{aligned} x_k &= \tilde{x}_k + \xi_k, \\ \xi_k &= \frac{c\mathcal{K}}{2} H^{-1} \eta_k \quad \left(= -\frac{c\mathcal{K}}{2} \eta_k H^{-1} \right), \\ \tilde{x}_k &= x_k - \frac{c\mathcal{K}}{2} H^{-1} \eta_k \quad \left(= x_k + \frac{c\mathcal{K}}{2} \eta_k H^{-1} \right), \end{aligned} \right\} \quad (k = 1, 2, 3). \quad (9)$$

One sees directly that ξ_k is odd. One examines the commutator of \tilde{x}_k with H :

$$\begin{aligned} H \tilde{x}_k - \tilde{x}_k H &= H x_k - x_k H - \frac{c\mathcal{K}}{2} \eta_k - \frac{c\mathcal{K}}{2} \eta_k, \\ &= \kappa c \alpha_k - c\mathcal{K} \eta_k = c\mathcal{K} \cdot cH^{-1} p_k. \end{aligned}$$

One sees that the *second* commutator vanishes, so \tilde{x}_k is even.

The ξ_k are “very small operators.” One easily calculates ⁽¹⁾:

$$\xi_k^2 = \frac{h^2 c^2}{16\pi^2} H^{-2} (1 - c^2 H^{-1} p_k^2). \quad (10)$$

It follows that the expectation values of ξ_k^2 , and thus, its eigenvalues, as well, are $\leq \left(\frac{h}{4\pi mc} \right)^2$. The eigenvalues of ξ_k itself are then (when one takes absolute values) $\leq \frac{h}{4\pi mc}$; i.e., the so-called Compton wave length, which is $\approx 10^{-11}$ cm. The x_k are then even “in the main.”

We shall now address the derivation of the decomposition of any function of the operators x_k from the decomposition of those operators; for example, of:

$$\frac{1}{r} = (x_1^2 + x_2^2 + x_3^2)^{-1/2}.$$

A general theorem about that can be stated. It reads thus: If:

$$f(a, b, c, \dots)$$

is an analytic function of the operators a, b, c, \dots , and if the decompositions of a, b, c, \dots are these:

$$a = g + u, \quad b = g' + u', \quad c = g'' + u'', \quad \dots$$

then the even part of $f(a, b, c, \dots)$ will be:

⁽¹⁾ These Sitzungsberichte, 17 July 1930; eq. (18).

$$\left. \begin{aligned} & \frac{1}{2}(f(g+u, g'+u', g''+u'', \dots) + f(g-u, g'-u', g''-u'', \dots)), \\ \text{and the odd part :} & \\ & \frac{1}{2}(f(g+u, g'+u', g''+u'', \dots) - f(g-u, g'-u', g''-u'', \dots)). \end{aligned} \right\} \quad (11)$$

The proof leads one to see that:

1. The theorem is correct for:

$$f(a, b, c, \dots) = a.$$

2. If it is true for $f(a, b, c, \dots)$ then it will also be true for the product of $f(a, b, c, \dots)$ and d :

$$f(a, b, c, \dots) d.$$

It then follows from this that it will be true for an arbitrary product of powers of any operators a, b, c, \dots , and thus, for any analytic function of any operators, as well.

That implies the following decomposition of $1/r$, or, to say the same thing, for K , the HAMILTONIAN operator of the hydrogen atoms [see equation (6)]:

$$\left. \begin{aligned} K &= G + U, \\ G &= H - \frac{e^2}{r} \left(r^{-1} + \left\{ \sum_{k=1}^3 (x_k - 2\xi_k) \right\}^{-1/2} \right), \\ U &= -\frac{e^2}{r} \left(r^{-1} + \left\{ \sum_{k=1}^3 (x_k - 2\xi_k) \right\}^{-1/2} \right). \end{aligned} \right\} \quad (12)$$

§ 4. We have now cleanly dissected the enemy. The operator U is the one that affects the mixing of negative functions with the hydrogen eigenfunctions, which makes it impossible to be completely free of them. However, the solution to the complication is now amazingly simple: *One can simply drop U and regard G as the Hamiltonian operator of the hydrogen atom without altering the hydrogen structure noticeably.*

If one were to argue in terms of the order of magnitude of U then one would not expect that. U obviously has the order of magnitude:

$$\frac{2(\xi_k)}{(r)} \approx \frac{h}{2\pi mc} \cdot \frac{4\pi^2 mc^2}{h^2} = \frac{2\pi e^2}{hc} = f,$$

in comparison to $e^2 / 2r$ (i.e., in comparison to the *energy of the term*). $[(\xi_k), (r)]$ shall denote the *orders of magnitude*. (r) is set to the radius of the innermost hydrogen orbit. f

is SOMMERFELD's fine structure constant, 0.00729.] If U were to provoke a perturbation of that order of magnitude then one could not remove U without disturbing the agreement with the observed fine structure completely, since it is known to have order of magnitude f^2 in comparison to the value of the term. The point is that an *odd* operator can provoke only *second-order* perturbations of the eigenvalues of G (as can subsequently be proved at once). In the present case, that does *not* mean, say, perturbations of order f^2 in comparison to the value of the term, which would still be inadmissibly large. Moreover, the perturbation operator must be compared to the *total energy* of order magnitude mc^2 . The former must have order f^2 compared to the latter, since the value of the term itself has only order $f^2 mc^2$. The *second-order* perturbations will then be only of order $f^2 mc^2$, or f^4 times the value of the term. That is much, much smaller than the fine structure, and it is even small in comparison to the natural line width (f^3 times the value of the term).

The supplementary proof that U can bring forth only second-order perturbation of the eigenvalues of G rests upon the fact that G itself differs from the field-free operator H only by a relatively-small perturbation with a relative order of magnitude f^2 . For that reason, one can be certain that G , just like H , possess only positive eigenfunctions for positive eigenvalues and only negative eigenfunctions for negative eigenvalues; or, in other words, that the case that was known to be possible at the end of § 2, for which positive and negative eigenfunctions belong to the same kinds of eigenvalues, is certainly *not* present for G . If a positive eigenvalue G' of G were to now belong to the s everywhere-positive eigenfunctions $\psi_1, \psi_2, \dots, \psi_s$ then the matrix of s^2 quantities:

$$\int \psi_\rho^* U \psi_\sigma d\tau \equiv 0$$

would vanish identically, since ψ_ρ is positive and $U\psi_\sigma$ is negative. The perturbation of the eigenvalue will then vanish to first order. Q. E. D.

§ 5. One convinces oneself, in entirely the same way, that the Stark effect of first and second order will not change noticeably when one drops the odd part of the additional field operator that represents the homogeneous electric field from the wave equation. The order-of-magnitude ratio between the even and odd parts will then be the same as it was for the central COULOMB field. One can then combine the two fields and see, with no further assumptions, that: Even when the external field is strong enough that a splitting of the order of magnitude of the value of the term comes about, the perturbation that is due to the odd part will remain less than the natural line width, just as before.

Things are somewhat more delicate for the Zeeman effect. If \mathfrak{A}_k are the components of the vector potential then the extra magnetic terms will have the form:

$$e \sum_{k=1}^3 \alpha_k \mathfrak{A}_k . \quad (13)$$

From (11), the decomposition of the vector potential is:

$$\begin{aligned} \text{Even part} &= \frac{1}{2} \{ \mathfrak{A}_k(x_1, x_2, x_3) + \mathfrak{A}_k(x_1 - 2\xi_1, x_2 - 2\xi_2, x_3 - 2\xi_3) \}, \\ \text{Odd part} &= \frac{1}{2} \{ \mathfrak{A}_k(x_1, x_2, x_3) - \mathfrak{A}_k(x_1 - 2\xi_1, x_2 - 2\xi_2, x_3 - 2\xi_3) \}. \end{aligned}$$

The \mathfrak{A}_k are therefore even, for the most part, while the odd part again has order of magnitude f in comparison to the even one (if one imagines that the order of magnitude of the x_k is the lowest orbital radius, as we always do here). However, *the even case is inverted* for the α_k . As we saw above, they are odd, in the main, and indeed the ratio of the components is equal to that of the macrovelocity to the speed of light; hence, the lowest hydrogen term is again f , but it is the *even* part that is small.

The same thing will then be true of the entire magnetic potential term (13). It is odd, for the most part. Nevertheless, from the DIRAC equation, the linear Zeeman effect will originate, for the most part (but not exclusively) in the *even* part of the operator (13).

If one next drops all *odd* components from the Hamiltonian operator, then the *even* part of (13) might provoke a magnetic perturbation (linear Zeeman effect) that has order:

$$f^s \tag{14}$$

(compared with the total energy mc^2). One now adds all odd terms at once. There are terms of order:

1. f^3 from the central field,
2. f^{s-1} from the magnetic field.

However, they act only quadratically. That gives three further perturbations, namely, in addition to the f^6 that was investigated before, two more perturbations of order:

$$\left. \begin{aligned} 1. & f^{s+2} \quad \text{for the linear Zeeman effect,} \\ 2. & f^{2s-2} \quad \text{for the quadratic Zeeman effect.} \end{aligned} \right\} \tag{15}$$

If we perhaps demand that both perturbations should remain restricted to the domain of the natural line-width (f^5) then the two inequalities:

$$s + 2 \geq 5, \quad 2s - 2 \geq 5$$

should be fulfilled, the second of which is more far-reaching, and demands that:

$$s \geq 3 \cdot 5.$$

From (14), that corresponds to a Zeeman effect that, after all, amounts to $f^{-1/2}$ (or about ten) times the fine-structure splitting.

It is only for very strong splittings that one can decisively prove anything for a quadratic Zeeman effect. Then, if the estimated orders of magnitude (15) are actually attained here, as above, then the *quadratic* Zeeman effect must prove to be roughly f^{-2} , and thus around 2×10^4 times greater in DIRAC's theory than it is for the modification that was proposed here.

§ 6. The provisional formulation of our attempt to separate the positive and negative wave functions is this:

One must restrict the Hamiltonian operator in the DIRAC equation to its *even* part by simply dropping the odd part.

Most likely, this formulation is still not conclusive. The next question that presents itself, and which I have still not been able to resolve up to now, is this: How does the altered equation behave in relation to the invariant-theoretic viewpoint? Is it Lorentz-invariant? Is it gauge-invariant? (One usually refers to “gauge invariance” when one means the obvious requirement that physical statements must not change when one employs one four-potential instead of another when they differ by only a four-dimensional gradient, because only the four-dimensional *rotation* of the potential – viz., the field strength – has any physical meaning.)

Here, one is not dealing with a purely mathematical question. Namely, it seems quite questionable whether the “electron coordinates” should refer to the eigenvalues of x_1, x_2, x_3 , and not those of $\tilde{x}_1, \tilde{x}_2, \tilde{x}_3$. In fact, with the $x_k = \tilde{x}_k + \xi_k$, the quantities $x_k - 2\xi_k = \tilde{x}_k - x_k$ seem largely equivalent. As I have learned from a friendly communication by J. v. NEUMANN, they can go to each other by a canonical transformation that takes every operator $g + u$ to $g - u$.

It then seems questionable whether the Lorentz transformation should be regarded as the well-known substitution of the eigenvalues of x_1, x_2, x_3 , and the parameter t , as before, or the substitution of the eigenvalues of $\tilde{x}_1, \tilde{x}_2, \tilde{x}_3$, and the parameter t . Moreover, in regard to that, I would like to prove that the mathematically clear and simple concept of a Lorentz transformation raises a truly significant difficulty from the quantum-theoretical standpoint: One prefers to assume that the coefficients of a Lorentz transformation are known precisely. Hence, one assumes that the relative velocity of two coordinate systems is known precisely. However, from the HEISENBERG uncertainty principle, their relative position will be completely indeterminate from that. Naturally, one can approach that difficulty in a purely-mathematical way when one imagines two sufficiently massive and absolutely rigid systems. However, from the physical standpoint, one must realize that nothing of that kind exists in reality, nor can it.

Received on 24 February
