Coup d'Etat: The Marginalization of the State in Quantum Field Theory

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1st May 2014

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Learning quantum field theory (QFT) for the first time, after first learning quantum mechanics (QM), one is (or maybe, rather, I was) struck by the change of emphasis: The notion of the quantum state, which plays such an essential role in QM, from the stationary states of the Bohr atom, over the Schrödinger equation to the interpretation debates over measurement and collapse, seems to fade from view when doing QFT. Not that it's gone - as any physicist will be quick to tell you, QFT is simply a quantum theory, with all the general structure between QM taken over unchanged. But it's hardly discussed, when dealing with Feynman diagrams, path integrals and all the other mainstays of an introductory QFT course.

This was not always so: The QFT of the late 1920s and 1930s developed as a straightforward extension and generalization of QM, and consequently writing down Schrödinger equations and calculating the energies of stationary states were the prime concerns of the physicists working with QFT at the time. But, as is well-known, this early QFT suffered from crippling defects, most notably the divergence problem, that all calculations appeared to give nonsensical, infinite results, once one went past the first approximation. These difficulties led to a multitude of attempts at revolutionizing the quantum theory of fields in the 1930s and 1940s. After the divergence difficulties of QFT (or at least of quantum electrodynamics) were solved through the renormalization techniques developed in the late 1940s, these more radical attempts were generally viewed as having gone way too far: Demanding a total overhaul of the foundations of the theory, when in fact small, conservative modifications were all that was needed in order to construct a workable QFT.

But, as I will argue in this paper, the form taken by the new, covariant and renormalized QFT can be understood a lot better, if one considers its origins not just in QM, but also in the failed attempts at a new quantum theory of fields of the 1930s and 1940s. In particular, the marginalization of the notion of the quantum state in the new QFT has its origins in two of these attempts, Heisenberg's S matrix theory and Wheeler-Feynman electrodynamics. These two attempts at a new theory were very different, but they shared one central aspect: They attempted to solve the difficulties of QFT, by getting rid of the notion of a (quantum) state altogether. Although this ultimately turned out to be going too far, the techniques and insights developed in the elaboration of these radical reworkings of QFT were taken over into "regular" QFT in the late 1940s, and defined the theory in an essential way. In particular, they allowed the physicists of the time to bracket highly problematic questions concerning the state space of QFT.

1 The S Matrix

Let us begin, by discussing the first of these failed attempts at a radically new QFT: Heisenberg's theory of the S matrix, laid out in a series of paper published during World War II. But let us go back even further, to study the origins of this theory in Heisenberg's attempts at incorporating a smallest, fundamental length into quantum theory. The fact that Heisenberg's S matrix has its origins in his theory of the fundamental length has often been remarked. In the following, I will be discussing this development specifically with an eye to the abolishment of the quantum state.

1.1 Heisenberg and the fundamental length

The development of Heisenberg's work on a fundamental length is described in [Kragh 1995]. The important point for our purposes is that initially the fundamental length was intended solely to remove the divergence difficulties of QED, acting as a cutoff scale for the divergent integrals appearing in higher order calculations in perturbation theory. The fundamental length was introduced into the theory by modifying the Hamiltonian, first by replacing differentials by differences (the 1930 lattice world, discussed in detail in [Carazza and Kragh 1995]), later by smearing out the energy density at a point in space with the help of a regularizing function (the 1935 Δ formalism, discussed in [Miller 1994]). These attempts always implied absolute limits on position measurements (or the measurements of field strengths at a point in space), but did not alter the general structure of the fundamental dynamical equations and held on to Hamiltonians and wave functions. These attempts did not go very far, running afoul, e.g., of their lack of relativistic invariance, and neither of them was ever published.

In 1936, Heisenberg turned to Fermi's theory of β decay, which implicitly contained a parameter with the units of a length in the form of the dimensionful coupling constant g. Initially, Heisenberg's interest in Fermi theory (as laid out in a letter to Pauli on 26 May 1936 [Hermann et al. 1985]) was not related to the divergence difficulties. Instead, he hoped that the dimensionful coupling constant of Fermi theory would help to explain the occurrence of cosmic ray showers.

What exactly was there to be explained? The difficulty was that the showers seemed to emanate from a single point, implying that all of the secondary particles were created in a single event. In QED, the creation of a large number of particles (photons and electron-positron pairs) in a single, localized event was very improbable: The more particles are involved in a single electromagnetic process, the higher powers of the fine structure constant $\alpha = e^2/\hbar c$ appear in the rate of said process, thus making the probability of a single explosive shower event incredibly small.

Heisenberg now realized that in Fermi theory the expansion parameter in a perturbative calculation is not simply proportional to the the equivalent of the fine structure constant, $g' = g/\hbar c$, which by itself is still dimensionful, but also to a power of the total momentum k involved in the process.[1] Heisenberg argued that for large momenta, the expansion parameter

[1]Which power depends on the formulation of Fermi theory one is using. Heisenberg was at the time considering the Uhlenbeck-Konopinski version, which includes an additional factor of neutrino momentum, so that the third power of the momentum enters the expansion paramenter.

also gets large and the situation is very different than in QED: many-particle processes become just as probable as one- or two-particle processes.

> It thu seems to me as though one could understand the existence of cosmic ray showers directly from Fermi's β theory.

Now, at first this seems to be totally unrelated to Heisenberg's earlier work on the fundamental length. That he was thinking of a connection already at the time of the quoted letter to Pauli, can be surmised from the fact that he chose a system of units (by introducing the necessary factors of $\hbar c$), where the coupling constant g' has the units cm^3, so that the expansion parameter is g'/λ^3, where λ is the wavelength of the incoming particle. This implied a reading where the explosive cosmic ray showers occurred when the wavelength of the exploding particle became greater than a critical length $\sqrt[3]{g'}$, where the expansion coefficient becomes of order one.

I have, and will be, distinguishing between the terms "fundamental length," to denote a length scale below which the usual notions of space no longer apply, and "critical length," to denote a length scale below which certain phenomena (e.g., explosions) occur. With the discovery of the critical length in Fermi theory, it was certainly tempting to connect this with the idea of a fundamental length. However, the critical length of Fermi theory was as yet unrelated to the problem the fundamental length had been supposed to solve: The divergence difficulties of QFT.

Pauli's reply is not extant, but he appears to have addressed precisely this point: Fermi theory diverged at higher orders of perturbation theory, just like QED did, so it was not permissible to explain cosmic ray showers through such higher order calculations. But Heisenberg was not to be deterred, and in his reply to Pauli on 30 May 1936 insisted on the differences between Fermi theory and QED: In QED the expansion parameter was small, so perturbation theory should work, but doesn't. In Fermi theory, on the other hand, the theory itself already indicated that perturbation theory should break down for high energies, so the divergence difficulties were not a defect of the theory as a whole, but only of the perturbative calculations:

> The non-convergence of the self-energy for large momenta in Fermi's theory is therefore not an argument against the theory, but - as long as one does not develop new mathematical techniques to treat the domain of high energies - only an argument for the lack of mathematical understanding of the calculating physicist. I do not claim that I am already sure that all self-energy difficulties will disappear in the future. But I do want to claim that all arguments so far concerning the infinite energies in the Fermi theory were nonsense and that it is now the most important task to check, how such a theory behaves qualitatively for high energies. To check this in quantum electrodynamics, however, would be pointless, since one knows that for dimensional reasons ($\frac{e^2}{\hbar c}$)) there is no qualitative difference between high and low energies.

The critical length thus did not function as a cutoff scale, as the fundamental length had. Instead, Heisenberg argued, for a theory including a critical length in the form of a dimensionful coupling constant, which was thereby able to qualitatively explain the cosmic ray explosions, one could hope that the divergences might simply be an artifact of perturbation theory. But this was very hard to verify, given that perturbation theory was the only known way to do calculations in QFT. Pauli and Heisenberg made some attempts at doing their calculations in discretized space, i.e., on the lattice (now just as a calculational tool, not as a model of physical space, as in 1930), but their results were inconclusive. Pauli became skeptical of the whole approach early on and became convinced that one could not construct a theory that was simultaneously free of divergences and able to describe explosions (Letter to Heisenberg, 26 October 1936):

> [S]o it always seems to be the case that *as soon as we have an increase of shower processes for large k , the eigenvalues of the Hamilton operator will also always come out infinite* [...]

By the end of the year, Heisenberg gave in and gave up, not just on the lattice, but on QFT as a whole. Already when originally proposing his idea of explosions and a fundamental length in Fermi theory, he had anticipated (Letter to Pauli, 30 May 1936):

> Of course, it is also conceivavle that the formalism of wave quantization will have to be modified when introducing Fermi's g, just like one had to modify the earlier physics when introducing the universal dimensionful constants c and h.

And this was the position to which he now again retreated (Letter to Pauli, 7 December 1936):

> I am now again totally convinced that the quantization rules are in need of reform [...]

What were to be the elements of a new theory, which renounced the quantum theory of fields which had, despite its apparent difficulties, matured in the last decade? This is the theme that we will now be following up until the formulation of S matrix theory.

One element that certainly remained was the critical length, which was to be related to the occurrence of explosive cosmic ray showers. This was now wedded to Heisenberg's earlier notion of a fundamental length, which provided absolute limits on measurement, a connection which had not been made explicitly, while Heisenberg still hoped to show the non-perturbative finiteness of Fermi theory. The connection between critical and fundamental length could in fact be made independently of all formalism through a physical argument by Bohr. It is first found in writing in a letter to Dirac, dating from 2 July 1936. Since Heisenberg had presented his work on the critical length in Copenhagen just a week earlier, it is quite probable that Bohr had communicated similar thoughts to Heisenberg himself:

> [T]hese new and most promising considerations of Heisenberg appear to me to offer a most important clue to the old problem of the limitation of the very ideas of space and time imposed by the atomistic structure of all measuring instruments. You may remember that we have often discussed such questions but hitherto it seemed most difficult to find an unambiguous starting point. It now appears,

> however, that any measurement of such short lengths and intervals where the conjugated momenta and energy will cause all matter to split into showers will be excluded in principle.

The same argument later shows up in published work of Heisenberg's, in which he also explicitly acknowledges discussions with Bohr [Heisenberg 1938]. The conclusion was: The critical length of explosion theory was also a fundamental length, because when trying to measure at scales smaller than the critical length, the measuring apparatus literally blew up in your face.

With this conceptual foundation, what was the formal basis on which Heisenberg continued his work? As witnessed by his last quote, his final disillusionment with QFT was directed at a very specific point of the theory, namely, the quantization, i.e., the transition from the classical to the quantum field theory. This meant that he believed that the unquantized Fermi field theory (including, in particular, the non-linear terms with the dimensionful coupling constant) was to be considered a correct basis for a future quantum theory (a hypothesis which he backed up by some semi-classical calculations on the creation of showers in [Heisenberg 1936]), but that the manner in which such a quantum theory was constructed from it, had to be rethought. On 18 December 1936 he wrote to Pauli:

> The current situation in field theory can be described in the following manner: We have a *korrespondenzmäßige* theory, which is about as good and as bad as Bohr's theory was at the time. In this approximate ("semi-classical") theory, the universal length is already *correctly* included, if one writes it as the factor multiplying a non-linear interaction term in the Hamiltonian. What is missing is the step from here to a consistent theory.

The analogy with the situation before the creation of quantum mechanics at this time becomes a recurring theme, and it will not be the last time we encounter it. That nostalgia for the revolution of their youth drove the protagonists of the creation of quantum mechanics to look for far too radical solutions to the woes of QFT is a cliché, but certainly has some truth to it. It even guided their search for solutions in even more specific ways: QM, according to matrix mechanics, was to be a discrete, algebraic theory. This vision was undermined by the triumph of Schrödinger's differential equation. Devising a new quantization procedure for field theory, now offered the possibility of undoing this historical error. Outlining his vision of a new quantization procedure, Heisenberg further wrote:

> [T]he particles of the future theory will not be smaller than the universal length, it will not even by possible to talk of a local interaction with a precision greater than the universal length (for example, I do not see the necessity for having a differential equation for ψ) [...]

To which Pauli remarked in the margins: "Lorentz Group." Relativity remained the bugbear of the fundamental length, as it had already been in 1930. In fact, it might well be argued that relativity already was the bugbear of matrix mechanics: Aside from a few awkward attempts by Dirac to turn time into a matrix, the union of quantum mechanics and relativity only began in earnest when the Schrödinger equation opened up the possibility of constructing generalized, relativistic wave equations.

1.2 The Beginnings of S Matrix Theory

Heisenberg's program was now the following: Reformulate QFT in such a manner that the Lorentz invariance was more clearly apparent; the usual methods, starting from Heisenberg and Pauli's initial formulation of 1929 were not explicitly covariant and relativistic invariance needed to be proven in quite a roundabout manner. Ideally, this reformulation should move away from the usual Schrödinger equation, which Heisenberg felt would have no place in the future theory. The reformulation would then be modified by integrating the fundamental length in such a manner that the equivalence with the regular Schrödinger equation was lost, thereby establishing a new quantization formalism that no longer relied on continuous functions and differential equations, but still guaranteed relativistic invariance.

It was already well-known that QFT could be formulated in a (more) covariant fashion by moving to the interaction picture. This had been established in 1932 in the works of Dirac, Rosenfeld, Vladimir Fock and Boris Podolsky [Dirac 1932; Rosenfeld 1932; Dirac et al. 1932]. The interaction picture by itself did not provide full relativistic invariance: This necessitated also the introduction of Dirac's many-time formalism, which, however, worked only for a finite number of electrons and not for hole or electron-positron theory. This defect was only cured by Tomonaga's introduction of super-many-times theory in 1943 [Tomonaga 1946]. In 1937, the central dynamical equation of the most covariant formulation of QFT was the Schrödinger equation (as given in the letter from Heisenberg to Pauli, 16 January 1937):

$$i\frac{\partial \varphi}{\partial t} = \overline{H_1}\varphi = \left(\int H_1 dV\right)\varphi \tag{1}$$

where H_1 is the Hamiltonian density in the interaction picture, i.e., just the interaction term, which is a relativistic invariant. The equation itself, however, is plainly non-covariant, since it makes explicit reference both to time and to space (in the volume integral).

It should be noted that the interaction picture, as introduced by Dirac, only had a time-dependent (and no time-independent) Schrödinger equation. This explains Heisenberg's starting point - in his entirely non-covariant 1929 formulation with Pauli, they had taken the time-independent Schrödinger equation as the central equation. In addition, his central concern at the time was scattering processes in cosmic rays (the explosions), something which could be addressed with a time-dependent Schrödinger equation, even if the usual treatment (see, e.g., the second, 1935, edition of Dirac's textbook [Dirac 1935]) relied on the time-independent Schrödinger equation. We see here for the first time, how demands of relativistic invariance joined with a new experimental focus (from the spectroscopic data of the first decades of the 20th century to the cosmic ray physics of the 1930s) to move the theory from the stationary to the dynamical. As to what this meant for determining the energies of stationary states, we will return to this question soon.

For now, Heisenberg now set himself to rewriting this equation, using the time evolution operator for an infinitesimal evolution dt:

$$\varphi(t+dt) = e^{-i\left(\int H_1 dV\right)dt}\varphi(t) = \prod_V e^{-iH_1 dV dt}\varphi(t) \tag{2}$$

where in the last step, Heisenberg used the notion of the integral as an infinite (Riemann) sum, to factorize the exponential, as well as the fact that the operators H_1 at different points in space commute. This could then be generalized to non-infinitesimal time evolution, by letting the product go not only over all of space, but over the entire space-time volume Ω between initial time t_0 and final time t_1:

$$\varphi(t_1) = \prod_{\Omega} e^{-iH_1 dx dy dz dt} \varphi(t_0) = \prod_{\Omega} e^{-iH_1 d\omega} \varphi(t_0) \tag{3}$$

where $d\omega$ is the space-time volume element. This equation even allowed, as Heisenberg hinted at in his letter, to take Ω as the volume between two arbitrary space-like surfaces, thereby achieving a fully covariant formulation. This is doubtlessly a very elegant procedure, foreshadowing the introduction of space-like surfaces by Tomonaga and Schwinger a decade later. Pauli was enthused (Letter to Heisenberg, 19 January 1937): "I find your equation [...] very pretty."

But, of course, it is still simply a reformulation of the regular Schrödinger equation. Heisenberg had high hopes that it might provide the right starting point for the development of a new quantization procedure, which also took account of the fundamental length. His program was to modify the time-evolution operator, in order to get a theory which remained relativistically invariant and was divergence-free. These modifications did not involve the fundamental length directly. As we have seen, Heisenberg believed that the fundamental length would already appear in the classical (Fermi) field theory and would then appear in the quantum theory in the correct manner, if one applied the new quantization procedure. The quantization procedure and the fundamental length were thus not necessarily connected.

Heisenberg's first attempt (January 1937) still involved the fundamental length, which would appear in the modified time evolution operator, mimicking the well-established but "scheußliche" cut-off procedures. These attempts soon floundered (Postcard to Pauli, 27 January 1937). Heisenberg's next attempt (February to April 1937) already no longer directly involved the fundamental length, and instead consisted in eliminating certain terms in the perturbation expansion of the time evolution operator, in order to avoid the divergences. Again, Heisenberg soon found the approach to be insufficient: It turned out to be impossible to simultaneously uphold relativistic invariance and remove the divergences (Letter to Pauli, 26 April 1937).

The details of these failed attempts need not concern us here. More important for us, are the general considerations which Heisenberg connected with these attempts (16 January 1937):

> [W]hat I like about the discussed proposal is that one gives up the notion of a "wave function at a certain position" and only introduces the notion of "a particle with a certain momentum."

This is a bit confusing: Heisenberg appears to be referring to the fact that the wave function φ is defined in occupation number space, rather than in (many-particle) configuration space. This was the usual procedure in QFT and made for much more tractable mathematics. However, the equivalence between the two formalisms was well-known and Pauli was consequently not so much confused, but rather, in typical Pauli fashion, enraged (19 January 1937):

I do *not at all* agree with the physical viewpoint that the notion "particle with a certain momentum" is physically better than the notion "wave function at a certain position". For the problem of the former notion is that one demands the momentum of the particle *at a certain, precise time* t (while momentum measurements can never be performed in an arbitrarily short time). Only in the force-free case, where the momenta are time-independent, is this not a problem; as soon as one has interaction terms, one has the same difficulties for $\varphi(N_k, M_k, t)$ [i.e., the wave function in occupation number space] as for $\varphi(x,t)^n$ [i.e., the wave function in n-particle configuration space].

As is often the case in the Heisenberg-Pauli correspondence, it is not entirely clear if Heisenberg had just been imprecise in his wording, or whether he only really thought things through after Pauli's harsh response to his half-baked musings. In any case, he responded on 21 January 1937:

I am, by the way, in total agreement with you that one can only speak of a precisely specified momentum for *free* particles, where the measurement can take as long as one wants. My considerations concerning $\prod_{\omega} e^{-iH_1 d\omega}$ [given the notation of his earlier letter, this should of course have been $\prod_{\Omega} e^{-iH_1 d\omega}$] actually had their starting point in the desire to replace this "differential" operator by an integral one, from which one can then only deduce cross sections for the transitions of free particles. But I have not been able to come up with a sensible generalization.

Since this is basically already the program for the S matrix, it is time to briefly take stock and consider again how Heisenberg arrived at this point. A combination of the demand for relativistic invariance (which was the central challenge for a theory of the fundamental length) and an interest in scattering processes, rather than spectroscopy, had led him to a formulation of QFT with the time evolution operator at its center. The next step was now supposed to be the move from the "differential" time evolution operator to an integral scattering operator. Such an operator would contain all that was necessary to describe a scattering event. It could of course be calculated in the regular QFT, based on differential equations, but would lead to divergent results. Heisenberg was now looking for a generalization, i.e., a modified calculational procedure, which could not be reduced back to differential equations, which Heisenberg felt were in conflict with a fundamental length. In particular, we see that the instantaneous state, in the form of a Schrödinger wave function, would be eliminated from such a theory, which would only speak about free asymptotic states.

Heisenberg did not further pursue this approach at the time. In fact, he entirely abandoned his attempts at a reformulation of QFT, after the first few had proven unsuccessful. In spring 1937, Heisenberg was increasingly on the defensive concerning the fundamental length and the theory of explosions. New experimental results implied that for low energies the supposed explosions could in fact be understood as electromagnetic cascades [Cassidy 1981]. Also, first hints were showing up that the high energy showers could be understood as resulting from the existence of "heavy electrons" and were also electromagnetic in nature (i.e., only involved photons, electrons, and positrons) [Galison 1983]. This invalidated Heisenberg's approach in a twofold manner: Nuclear forces (i.e., Fermi's theory of β decay) did not seem to be involved in shower production at all, and the showers were no longer viewed as single explosive events. It also became increasingly doubtful, whether the theory of β decay was to involve a dimensionful coupling constant at all, when the apparent confirmation Yukawa's meson theory implied that β decay was not actually a four-fermion interaction, but rather mediated by a heavy boson.

How did these developments affect Heisenberg's research program? The fundamental length and its manifestation in the form of cosmic ray explosions (which now, however, had to be taken as a lot less common than originally envisioned) remained cornerstones of Heisenberg's vision for a new theory. This is not true for the other tenet of Heisenberg's work in early 1937, that the correct semi-classical field theory was already known and one only needed to cook up a new and improved quantization procedure. As already mentioned, the fundamental nature of Fermi's theory of four-fermion interactions was increasingly called into doubt. At the same time, the meson theories which were supposed to replace it, also ran into ever greater difficulties. After an initial optimism, it became increasingly clear that they were unable to reconcile nuclear and cosmic ray phenomenology. This conundrum was only resolved after the war, with the conceptual separation between the original cosmic ray meson (the muon) and the carrier of the nuclear force (the Yukawa meson or pion).

When Heisenberg thus returned to attempts at constructing a new relativistic quantum field theory in the isolation of wartime, it was no longer with the aim of merely modifying the quantization procedure. Instead, the idea was now to construct a new theory from scratch. This brought his old idea of an integral scattering operator back on the table.

The motivations (elimination of states and differential equations in order to account for the fundamental length, central role of scattering processes in order to describe explosions) were still valid. And at the same time, his former difficulties were now moot: He had found himself unable to find a suitable generalization of the procedure which led from a correct semi-classical field theory to such an operator, a generalization which would eliminate the divergences which appeared in the usual quantization procedure. There was now no trustworthy semi-classical field theory to start from. Instead, Heisenberg now proposed to take the integral scattering operator (now S matrix) itself as the starting point of the theory.

This was a radical move away from the central ideas of quantum theory, which since Bohr's correspondence principle had always relied on relating classical and quantum theories in some way or another. It was to bring with it major difficulties, which we will discuss in detail. Above all, it needed a new philosophical underpinning. Here again, Heisenberg turned to the glory days of the creation of quantum mechanics. The positivist program of constructing a theory including only observable quantities, which he had laid out in the introduction to his 1925 "Umdeutung" paper, was in fact logically distinct from the idea of transferring mathematical structures from a corresponding classical theory. Heisenberg could thus divorce these ideas from the theory of quantum mechanics, to which they had originally led, and re-present them as the basis for his new S matrix theory, which was consequently published in a series of papers titled *Über die beobachtbaren Größen' in der Theorie der Elementarteilchen*" ("Concerning the observable quantities in the theory of elementary particles"). It is to these papers that we now turn.

1.3 Heisenberg's S Matrix Theory

The first thing one needs to note concerning Heisenberg's S Matrix papers, is that they do not constitute an actual, full-fledged physical theory. This can be immediately understood from the abandonment of the correspondence idea. In QM, one could write down the abstract Schrödinger equation

$$H\psi = E\psi \tag{4}$$

as a purely quantum equation, but it was the correspondence with a classical theory that provided the input on what sort of an operator H really was. One can learn a lot about the structure of QM without ever invoking a specific Hamiltonian. Heisenberg had something similar in mind for his S Matrix theory. Only now, the elements of the S matrix should be observables and have an immediate and clear physical interpretation, so that the general, structural insights into the new theory should be "at least in principle empirically testable." (I, p.514)

No direct physical predictions emerged from Heisenberg's work on the S Matrix, so this statement should be understood as attempting to reconcile the two almost contradictory aspects of this work: On the one hand, it is a mere formal scheme, on the other hand, it is supposed to be an expression of positivist empiricism, making reference only to observable quantities.

For the time being, Heisenberg had to leave open the question of how the scheme of S Matrix theory was to be filled with physical content. The more immediate question was what actually were to be the observable quantities on which the theory was based. Or rather, which quantities weren't observable. Heisenberg had learned his lesson from the debates following the *Umdeutung*. In 1926, he had presented his work in Berlin and had a discussion with Einstein, which had impressed him so much that he repeated it verbatim in his 1969 autobiography [Heisenberg 1969]. Einstein had said to him:

> [I]t may be heuristically useful, to remind oneself, what one is really observing. But from a fundamental standpoint it is entirely wrong, to want to build a theory only on observable quantities. For in reality it is exactly the other way around. It is only the theory that decides, what one can observe.

This sentiment, which is missing in the *Umdeutung*, is echoed in the introduction to Heisenberg's first S Matrix paper:

> [A]lso the future theory should of course primarily contain relations between "observable quantities." Of course only the final theory will determine, which quantities are really observable.

Now, there was no "final theory." This is where the fundamental length comes in:

> The existence of a "smallest length", i.e., of a universal constant of the dimensions of a length and of the order of 10^{-13} cm, makes problematic all of those statements of quantum theory, which deal with the precise determination of a position or of a point in time, i.e., with spatio-temporal processes in general.

Here is, in a nutshell, the argument for the abolishment of continuous fields and state functions, and the differential equations that govern their behavior. But what were the observable quantities, which the new theory would be based on, to be? Heisenberg named two. One of them was clearly the (cosmic ray) scattering cross sections, which were derived from the elements of the S Matrix and which were to describe, in particular, the occurrence of explosions. The other, and these could not be done away with, were the central observable quantities of the old theory, the energies of the stationary states.

Now, there seems to be somewhat of a contradiction here: On the one hand, the elevation of the scattering operator to the central entity of the new theory, with the concomitant abolishment of anything but asymptotic, free states. On the other hand, the wish to keep the central observable and calculable quantity of QM (and the QFT of the time), the energy of stationary states, which was, however, obviously closely tied to the notion of state, which was being abandoned. Heisenberg had felt this difficulty already in 1937 - at the time, he was still discussing the (differential) time evolution operator; but already here the discrepancy becomes apparent. On 14 February 1937, he had written to Pauli:

> Of course one still has to find a connection [...] to the magnitude of the rest mass and to the question of the stationary states. I have not been able to obtain such a connection so far; I only have a few tentative attempts, but I do not know, whether they will work out.

He voiced similar concerns in the first S Matrix paper, five years later:

> The two [...] kinds of observable quantities at first sight seem to be without inner connection, and one gets the impression that, for spatially enclosed systems with discrete eigenvalues on the one hand, and for non-enclosed collision and scattering processes with continuous energy spectrum on the other, one needs to treat entirely different quantities as “observable” .

But Heisenberg brushed away these concerns in 1943, and made a very vague claim concerning the equivalence of the two types of observables. Two years later Christian Møller disproved what he took to be Heisenberg’s claim: that “the discrete energy values in the closed stationary states are at least partly determined by the S-matrix.” He showed that this was not the case.

The proof was simple: Start from a scattering potential that allows both scattering and bound states (the classical example of course being a Coulomb potential). In QM this corresponds to a Hamiltonian with both continuous (scattering) and discrete (bound state) eigenvalues. Now, assume we have solved the scattering problem completely, i.e., determined all the eigenfunctions belonging to the continuous eigenvalues. This is of course a lot *more* information than is contained in the S-Matrix, which is only concerned with the asymptotic behavior of these eigenfunctions. Still, all this allows us to do is determine the eigenspace corresponding to the discrete eigenvalues of the Hamiltonian: It is the subspace of the total Hilbert space that is orthogonal to all the eigenfunctions belonging to continuous eigenvalues. But we can say nothing about which is the correct eigenbasis in this subspace, nor do we know anything about the corresponding eigenvalues. In other words, we have only partially diagonalized the

Hamiltonian, and in order to know the bound state energies we need to fully diagonalize, i.e., explicitly solve the bound state problem.

This argument is so simple that it is hard to believe that the statement being disproved is really what Heisenberg was claiming. And indeed, looking more closely at Heisenberg's claims of 1943, his claim does look somewhat different:

> [It] is to be taken as observable the behavior of the in- and outgoing waves at infinity; i.e., in particular the phase difference between the in- and outgoing spherical wave belonging to a certain angular dependence (i.e., to a certain angular momentum of the system). If the system is now enclosed by a spherical shell at a great distance, the energy values of the system become discrete. These energy values, however, only depend on the phase difference between the in- and outgoing wave. If one considers the energy values of the thus modified system to be observable, this is the same as taking the phase difference to be observable [...]

Heisenberg was thus not, as Møller read him, talking about the case where the QM Hamiltonian has both continuous and discrete eigenvalues at the same time. Rather, his starting point is an unenclosed system with continuous eigenvalues - he does not at all touch upon, whether there is a discrete part of the spectrum corresponding to bound states as well. Instead, he goes from this system to an enclosed system, in which the entire energy spectrum is discrete, and then argues that knowing the S-Matrix of the unenclosed system is equivalent to knowing the discrete energy spectrum of the enclosed system.

His argument, therefore, only applied, say, to the problem of a particle in an infinitely high potential well, but not to the more physical cases discussed by Møller, where the setup allows both for scattering and for bound states, such as a hydrogen atom. The general problem of bound state energies in a theory which did not deal in states was thus not addressed, even though Heisenberg's wording is very suggestive and certainly initially fooled Møller:

> *A priori* this seems possible, since the asymptotic form of the wave function in great distances which determines the collision cross sections, depends chiefly on the form of the potential function in small distances, which again is essential for the position of the discrete energy levels. (p.18)

Maybe Heisenberg even had himself fooled, since he entirely left out the question of bound state energies in his first paper, focusing only on developing the S Matrix formalism as a relativistically invariant description of scattering processes. He continued in the same vein in the second paper: Here he constructed an S Matrix which would lead to explosions, while at the same time being entirely finite. This S Matrix was of course not derivable from a Hamiltonian operator, and could thus not be regarded as the result of the quantization of any classical field theory. It described a "nicht korrespondenzmäßig deutbare Wechselwirkung," which was anyway not supposed to be a realistic model of nuclear interactions, for which Heisenberg would have had to go beyond cosmic ray scattering phenomenology and talk about nuclear bound state phenomenology (the deuteron was the classical test case for theories of nuclear interaction). But it furnished a proof of principle that the requirements he had set for a future theory already in 1936 could be met by an S Matrix theory.

Despite the war, Heisenberg's papers reached physicists all across the world, even his old pal Pauli in Princeton. Unable to communicate with Heisenberg directly, he instead voiced his usual criticism in a letter to Paul Dirac (21 December 1943), pointing out the two main difficulties of the S Matrix program:

> Heisenberg did not try to give any theoretical formalism which determines his matrix. Even if such a formalism can be found, other problems would still exist to which the S-matrix is not adapted, as for instance properties of stationary states of compound systems. (For instance the stationary-states of the deuteron as a consequence of the interaction of the protons and the neutrons with the meson-field.)

At about the same time, however, unbeknownst to Pauli, the second problem was being addressed in Europe by Heisenberg and Hans Kramers.

1.4 The Analytic S Matrix

Discovery of Analyticity to be filled in with help of the Heisenberg Papers.

2 Wheeler-Feynman Electrodynamics

As we have seen, Heisenberg's S Matrix program emerged first from attempts to modify the quantization procedure and then from attempts to construct an autonomous quantum theory, independent of a classical field theory. It can thus be placed in a school of thought that viewed the difficulties of QFT as stemming from the quantum theory proper. All through the 1930s and 40s there was another popular viewpoint, which viewed the divergence difficulties as an inheritance from classical theory. The proposed solution was thus a modification of the classical theory. Such attempts tended to focus less on the theory of nuclear interactions and more on electrodynamics, where the classical field theory and its difficulties were well-established. The most radical of these attempts tried to get rid of the electromagnetic field entirely.

2.1 Absorber Theory

This idea came to Richard Feynman, according to his own recollections, as an undergraduate student at MIT (1935-39), after studying QED in the standard textbooks of the time by Dirac and Heitler.[2] Interestingly, these two textbooks are good representatives of the two schools of thought introduced above. Heitler clearly argued for the quantum nature of the divergence difficulties (p. 183 of the second edition), while Dirac explicitly stated:

> The limitations in the applicability of quantum electrodynamics [...] correspond precisely to those of classical electrodynamics. The amendments required in clas-

[2] The following narrative is heavily indebted to [Mehra 1994].

> sical theory in order to make it applicable accurately to the elementary charged particles are thus not provided by the passage to the quantum theory...

While Feynman initially tended towards Dirac's view on this matter, it appears to have been Heitler's detailed elaboration of the origin of the divergences that directly influenced his search for a solution. Heitler identified two sources for the central divergent quantity, the self-energy of the electron. There is first the electrostatic self-energy, which is due to the self-force, "the force which the field produced by the charge exerts on the charge itself" (p. 29 of the second edition). And then there is the transverse self-energy, which is due to virtual photons in the intermediate states of higher-order perturbation calculations. It is divergent because "the number of intermediate states is infinite" (p. 184 of the second edition), i.e., because the electromagnetic field has an infinite number of degrees of freedom.[3]

As Feynman now recalls, the immediate solution to both of these problems seemed to be the abolishment of the electromagnetic field. This would eliminate the infinite number of degrees of freedom. The theory could then be recast as a theory of action-at-a-distance between electrons, where the action would have to be taken as retarded and not as instantaneous. This would allow the self-consistent elimination of the interaction of an electron with itself, which was not possible if the interaction was described through a universal field.

Although this was probably not the young Feynman's immediate priority, it is clear that already this general proposal problematizes the notion of an instantaneous state: For a retarded action-at-a-distance it is not sufficient to know the initial conditions and let them evolve. Rather, one needs to know a lot about the past evolution of the system. Such a setup thus, already classically, does not offer itself to a Hamiltonian treatment, which would provide the basis for the transition to the corresponding quantum theory.

When Feynman went to Princeton as a graduate student in 1939, his new advisor, John Wheeler, pointed him to a much more immediate problem in this approach. If one eliminated the action of an electron on itself, one not only got rid of the troublesome infinite electrostatic self-energy, but also of radiative reaction, i.e., the recoil experienced by an electron emitting electromagnetic radiation.

Together, Wheeler and Feynman thus modified Feynman's original proposal. They could show that if one replaced the retarded action-at-a-distance by a combination of retarded and advanced interactions (in field theory this would correspond to taking the average of the advanced and retarded electromagnetic potentials) one could include the radiative reaction: The radiative reaction emerged as the reaction of the emitting electron to the advanced back-reaction of all the other electrons in the universe, if one assumed that there were sufficiently many of these to ensure that all emitted radiation would eventually be absorbed (hence, Wheeler-Feynman electrodynamics is also known as absorber theory).

There remained the central difficulty of the mathematical formulation: Even more than in a theory of retarded interactions, a theory of advanced and retarded interactions could not be formulated as a Hamiltonian theory of the time evolution of instantaneous states. But

[3]Feynman recalled that, at the time, he mistakenly believed that the infinite number of degrees of freedom only showed up in the infinite zero-point energy. Both [Schweber 1994, p.379-380] and [Mehra 1994, p.89] read this as Feynman being mistaken on the whole difficulty of the infinite degrees of freedom, not taking into account that in the literature of the day the infinite degrees of freedom were made responsible not just for the zero-point but also for the transverse self-energy.

Wheeler happened upon a paper by the Dutch physicist Adriaan Fokker in which this difficulty was solved.

In 1929, Fokker had in fact constructed a formulation of the electrodynamics of point particles as a combination of advanced and retarded actions-at-a-distance. He had not been concerned with the question of the radiation reaction, but he had arrived at the same combination of advanced and retarded actions-at-a-distance merely through the demand of a relativistically invariant action functional [Fokker 1929b]. The formulation using the principle of least action avoided the difficulties of the Hamiltonian formalism: The entire world-lines (space-time trajectories) could be obtained from the minimization of the action functional instead of constructing them from inifinitesimal time evolution. In Feynman's notation, the Fokker action reads (for a set of electrons, labeled by an index a, with coordinates x_a, proper times τ_a, charges e_a, and masses m_a):

$$S = -\sum_a m_a c \int_{-\infty}^{\infty} \sqrt{-\dot{x}_a^{\mu}\dot{x}_{a\mu}}\, d\tau_a + \sum_{a<b} \frac{e_a e_b}{c} \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \delta\left(\left(x_a^{\mu} - x_b^{\mu}\right)^2\right) \dot{x}_a^{\nu}\dot{x}_{b,\nu}\, d\tau_a\, d\tau_b \tag{5}$$

When supplemented with the absorber initial conditions, this action provided an elegant reformulation of classical electron theory without involving the notion of a field. But this was of course only the starting point for the actual program: The construction of a new quantum electrodynamics. While Wheeler was constantly announcing that the quantization of the absorber theory was almost ready, while not communicating any of the details, Feynman pondered the question by himself, taking the Fokker action as his starting point.

Already Fokker had republished his work in German [Fokker 1929a] shortly after the publication of the original Heisenberg-Pauli QED, now presenting it as an alternative starting point for the construction of a quantum theory of electrodynamics. The full extent of the divergence difficulties had not yet been realized at the time, so Fokker's main argument for the superiority of his least action formulation was its manifest relativistic invariance. But Fokker did not pursue the quantization of his theory any further. An obvious reason is that, while Heisenberg and Pauli could rely on the established quantization procedures of QM, it was unclear how to construct a quantum theory from a classical theory which was only formulated using a least action principle. The emphasis here is on *only*. A general classical theory can of course also be written using the principle of least action, with an action functional of the form

$$\mathscr{A} = \int_{t_0}^{t_1} L(q, \dot{q})\, dt \tag{6}$$

with the Lagrangian L some function of the dynamical variables q and their time derivatives $\dot{q}$. From the Lagrangian one can then construct the Hamiltonian (leaving aside questions of gauge invariance, which forms an entirely unrelated difficulty) in the usual manner, which forms the starting point for canonical quantizations. But the Fokker action differs from this usual form in two decisive aspects. The first is that the integrations are over the proper times of all of the involved particles instead of over some universal time coordinate. The second is that the integrations are carried out from $-\infty$ to ∞, instead of from an initial time t_0 to a final time t_1.

It is this latter difficulty which is related to the central focus of this paper: For an action formulated in terms of a Lagrangian, the time integration range can be taken infinitesimally small. The action is then minimized in each infinitesimal step and thus the contact is made with the Hamiltonian formulation of differential time evolution of instantaneous states. This is not possible for the Fokker action: Since the interaction is retarded (and advanced), one always needs to take into account the entire trajectories. This is another way of stating that the notion of state is lost in such an action-at-a-distance theory.

Over a decade later, Feynman was faced with the same difficulty. But, different from Fokker, he could draw on the work of Paul Dirac, who had made some first steps towards the quantization of a classical theory formulated using the least action principle. It is to this work of Dirac's that we now turn.

2.2 Dirac's Lagrangian Quantum Theory

The relation between quantum theory and relativity is a *leitmotif* in the work of Paul Dirac. Early on, he attempted to reconcile matrix mechanics and relativity by elevating time to the status of q number. In 1928, he presented the relativistic generalization of the Schrödinger equation, certainly his best-known contribution to this problem context. In 1933, he presented another step towards a more relativistic quantum theory, his paper "The Lagrangian in Quantum Mechanics." Parts of this paper are then taken up in the second edition of Dirac's textbook. This seems to be Feynman's source: In his thesis, only Dirac's book is cited, the reference to the 1933 article (which was published in the *Physikalische Zeitschrift der Sowjetunion*) only appears as a "see also" in the 1948 article based on the thesis. We thus will only concern ourselves with the material reprinted in 1935 and not with the (even) more speculative parts of the paper, which concern the generalized transformation function and were also very influential, especially for the development of quantum field theory in Japan.

The starting point of this work is Dirac's dissatisfaction with the usual Hamiltonian formalism, but for a reason unrelated to Feynman's difficulty: Its lack of manifest covariance. Indeed, the Hamiltonian of a system is not a relativistic invariant, it is rather the time component of a four vector. Dirac was thus looking for a formulation of QM which was closer to the classical Lagrangian formalism, since the Lagrangian function *is* a relativistic invariant. This was, however, far from straightforward, as he outlined in the introduction to the 1933 paper:

> A little consideration shows, however, that one cannot expect to be able to take over the classical Lagrangian equations in any very direct way. These equations involve partial derivatives of the Lagrangian with respect to the coordinates and velocities and no meaning can be given to such derivatives in quantum mechanics. The only differentiation process that can be carried out with respect to the dynamical variables of quantum mechanics is that of forming Poisson brackets and this process leads to the Hamiltonian theory.
> We must therefore seek our quantum Lagrangian theory in an indirect way.

This indirect way relied on another role played by the Lagrangian in classical mechanics, besides its appearance in the Euler-Lagrange equations of motion, which result from the extremization of the action. The Lagrangian also appears in the expression for Hamilton's principal function S, that is the action functional $\mathscr{A}$ (Equation 6) evaluated on the actual, physical path. Since this path is obtained by extremizing the action functional, the principal function is the extremum value of the action functional. In the classical theory, this principal function, taken as a function of the beginning and end points of the trajectory, q_T and q_t, respectively, can now be viewed as the generator of a canonical transformation that connects the canonical variables at times T with those at time t, i.e.

$$\begin{aligned} p_t &= -\frac{\partial S}{\partial q_t} \\ p_T &= \frac{\partial S}{\partial q_T} \end{aligned} \tag{7}$$

Instead of introducing the Lagrangian into quantum mechanics via the equations of motion, as it was done for the Hamiltonian (be those equations of motion the Heisenberg picture equations of motion, which include the commutator of the Hamiltonian with a given observable, or the Schrödinger equation), Dirac could now introduce the Lagrangian through the relation between classical canonical transformations and quantum unitary transformations.

This relation was an important issue in the early days of matrix mechanics [Lacki 2004]. It was made obsolete by the establishment of transformation theory and modern quantum mechanics. Some questions were, however, left open, including the one at stake here: Given a classical canonical transformation what is the corresponding unitary transformation in quantum mechanics? Dirac attempted to give an answer to this question in 1933. His argument is, however, quite opaque. There is one thing that he unambiguously shows: Just as for classical canonical transformations, unitary transformations in quantum mechanics can also be expressed by a generating function (which is a function of the old and the new canonical coordinates, as was the case above). This is done in the following form: Let the scalar product between an eigenstate of the old canonical coordinates q with the eigenvalue q' and an eigenstate of the new canonical coordinates Q with the eigenvalue Q' is given by:

$$\langle q' \big| Q' \rangle = e^{iF(q',Q')/\hbar} \tag{8}$$

where F is some generating function. Dirac could then show that the matrix elements of the old and new canonical momenta (and imposing some restrictions concerning the ordering of operators, also the momentum operators) obeyed the classical transformation equations, which are of the form given above

$$\begin{aligned} \langle q' \big| p \big| Q' \rangle &= \frac{\partial F(q',Q')}{\partial q'} \langle q' \big| Q' \rangle \\ \langle q' \big| P \big| Q' \rangle &= -\frac{\partial F(q',Q')}{\partial Q'} \langle q' \big| Q' \rangle \end{aligned} \tag{9}$$

The decisive question is now: What is the relation between the classical and the quantum generating function? From Dirac's elaborations, both in the 1933 paper and the 1935 book, it appears that Dirac did not really consider this question. He introduces the generating function in the quantum theory as a distinct mathematical object, without giving any relation between the quantum and classical generating functions. They are merely treated as analogous. [4]

Applying this to the case of the classical time evolution canonical transformation discussed above, this implied that also in the quantum case, there would be a generating function related to unitary time evolution, which is (and this certainly adds to the confusion) also denoted by S and is given by

$$\left\langle q_t' \middle| q_T' \right\rangle = e^{iS(q_t', q_T')/\hbar} \tag{10}$$

where $|q_T'\rangle$ and $|q_t'\rangle$ are eigenkets of the canonical coordinate operators (in the Heisenberg representation) at the initial and final times. S can then be considered the quantum analogue of the classical principal function. Since the precise nature of this analogy is not defined, the only upshot of Dirac's study was that a quantum theory modeled more closely on the classical Lagrangian formulation would be based on the (transformation) matrix elements $\left\langle q_t' \middle| q_T' \right\rangle$, rather than on a quantum state evolving in time. Such a formulation could thus be a better starting point for a relativistic generalization of QM.

Dirac's program (which he himself did not pursue much further) was thus very similar to that of Heisenberg in early 1937: Rewrite quantum theory in a more explicitly covariant manner, in order to have a better starting point for obtaining the correct relativistic theory. And, indeed, they ended up at very similar formulations: Dirac's transformation matrix elements are simply the matrix elements of the Schrödinger (or interaction) picture time evolution operator, expressed in the Heisenberg picture. So, just like Heisenberg in 1937, Dirac's attempts at re-writing quantum theory in a more relativistic fashion, had led him to an approach in which the procedural took precedence over the study of stationary states.

What Dirac did not supply was any novel way of calculating these transformation matrix elements. The question of what the quantum generating function would be was left entirely open. It was Feynman who was to fill this gap, at the same time taking the step that Heisenberg had also taken, namely to move from a theory which still made explicit reference to arbitrary initial and final states of a process, to a theory in which only free, asymptotic states appeared and the notion of the differential evolution of an instantaneous state was gone. And in both cases, it was the attempt to solve the divergence difficulties of QFT which motivated this next step: For Heisenberg it had been the fundamental length, for Feynman it was action-at-a-distance electrodynamics.

[4] Indeed no general relation between quantum and classical generating functions was established by Feynman, who only deals with infinitesimal time translations. If equation 68 on page 113 of Dirac's book were intended to imply the general numerical equality of quantum and classical generating functions, it would be plain wrong - it would not even hold for finite time evolutions. But Dirac clearly identifies the S in this equation as merely denoting the quantum generating function. I therefore believe that Wüthrich's argument that Dirac here anticipated Feynman's work [Wüthrich 2010, p.53] is fallacious. Julian Schwinger's take on the whole question was the following: "Now, we know, and Dirac surely knew, that to within a constant factor the "correspondence" for infinitesimal dt is an equality when we deal with a system of nonrelativistic particles possessing a coordinate-dependent potential energy V. [...] Why, then, did Dirac not make a more precise, if less general, statement? Because he was interested only in a general question: What, in quantum mechanics, corresponds to the classical principle of stationary action ?" [Schwinger 1989]

2.3 Feynman's Path Integrals

Feynman's realization that there is a very close relation (indeed proportionality) between the classical and quantum generating functions for the special case of infinitesimal time evolution occurred in the Spring of 1941. The amusing anecdote of how he hit upon this fact, with the help of German physicist Herbert Jehle, is recounted by himself in his Nobel lecture. Using this fact, and iterating the infinitesimal time evolutions to obtain an expression for finite time evolutions, he arrived at his famous path integral formulation of (non-relativistic) quantum mechanics. The details of this discovery need not concern us here, they are discussed, e.g., in [Wüthrich 2010]. What Feynman ended up with was an expression for arbitrary matrix elements between an initial state ψ at time t_0 and a final state χ at time t_1. As a simplest case, this gives an expression for Dirac's transformation matrix elements, generalized to an arbitrary initial and final state:

$$\langle \chi(t_1) \big| \psi(t_0) \rangle = \int \chi^*(x_k, t_1) \exp\left[\frac{i}{\hbar} \sum_{i=0}^{k-1} L\left(x_{i+1}, \frac{x_{i+1} - x_i}{\epsilon} \right) \epsilon \right] \psi(x_0, t_0) \frac{dx_0}{A} \frac{dx_1}{A} \cdots \frac{dx_{k-1}}{A} dx_k \tag{11}$$

where

$$\epsilon = \frac{t_1 - t_0}{k} \tag{12}$$

is the infinitesimal time interval introduced through the iteration of the infinitesimal time evolution and A is a normalization factor. In the limit where ϵ is taken to zero, the familiar path integral arises, but Feynman eschewed the highly problematic notion of functional integration, both in his thesis and his first paper on path integrals in 1948. Still the limit of continuous time was conceptually important, because in this limit the sum in the exponential would be replaced by an integral (and the difference quotient in the argument of the Lagrangian by a time derivative), giving, and this was Feynman's second great insight, the classical action functional of equation 6.

This realization allowed Feynman to go beyond a mere reformulation (albeit a very elegant and hugely influential one) of regular non-relativistic QM to the quantization of theories which had no Hamiltonian, only an action. This had been, after all, his goal: To quantize the absorber theory starting from the Fokker action.

Here now, in discussing in general the quantization of a classical theory with only an action, Feynman really began to wrestle with the difficulty of the absence of states. For after all, the matrix elements when calculated in the action method for physical systems with a regular Lagrangian, still explicitly depend on the initial and final quantum mechanical states at some finite times t_0 and t_1. Feynman's solution was to assume that the non-Lagrangian nature of the system only existed for a finite time:

> This difficulty may be circumvented by altering our mechanical problem. We may assume that at a certain very large positive time T_2, and at a large negative time T_1, all of the interactions (e.g., the charges) have gone to zero and the particles are just a set of free particles (or at least their motion is describable by a Lagrangian).

> We may then put wave functions, χ and ψ, for these times, when the particles are free, into [the equation for the matrix elements]. (We might then suppose that the motion in the actual problem may be a limit of the motion as these times T_1 and T_2 move out to infinity).

Feynman thus, just like Heisenberg, arrived at the point where the theory could only speak about transitions between asymptotic free states, while the evolution of the state in some intermediate area of interaction was inaccessible to the theory. This establishment of this view may be viewed as stemming from philosophical preferences. Indeed, Feynman himself in his Nobel lecture stated that at this time he developed a preference for an "overall space-time point of view," where one always only considered the full evolution of systems, and a "disrespect for the Hamiltonian method of describing physics," where "things are discussed as a function of time in very great detail." Schweber [Schweber 1994, p. 393] also claims that Feynman's recasting of QM was "clearly influenced by the S-matrix viewpoint Wheeler had expounded to him."

What is this "S-Matrix viewpoint" of Wheeler's? For one, Wheeler was the first one to use the S-Matrix -years before Heisenberg, in 1937, though Heisenberg claims he developed the idea independently [Rechenberg 1989], which is plausible, given that he had already arrived at the idea of an integral scattering operator in 1937. In any case, for Wheeler the S matrix was merely a calculational tool in non-relativistic nuclear physics and not the central quantity of the current or a future theory. Rather, Schweber is referring to a view of Wheeler's "that all quantum-mechanical descriptions of physical phenomena could be construed as scattering processes" [Schweber 1994, p. 379]. Wheeler jokingly referred to these ideas of his as "everything as scattering," and they most certainly influenced Feynman's diagrammatic approach to perturbation theory. But these developments were still far off in 1942, and Wheeler himself placed his work on Wheeler-Feynman electrodynamics in the context of a different, albeit similarly ambitious, program of "everything as electrons." [Wheeler 1989] Also, the idea of "everything as scattering" is clearly distinct both from Heisenberg's philosophical starting point of reducing everything to observables (which played no apparent role for Feynman) and from Feynman's own space-time point of view. So, while such general philosophical considerations certainly played a role for all the involved actors, they do not explain the surprising convergence of the programs of Heisenberg and Feynman.

The common origin of their arrival at a theory that only connects free, asymptotic states is rather the belief that the failure of QED should be understood from the misguided ambition of giving a detailed picture of infinitesimal time development. Their reading of why such a picture is impossible is very different (fundamental length v. action-at-a-distance), but the conclusions are strikingly similar. It is indeed probable that Feynman was driven to the adoption of his viewpoint by the difficulties of QED, rather than by some overarching philosophical program. Schweber himself cites another interview with Feynman that Schweber himself conducted (p. 396):

> The reason in my philosophy not to descend to the Schrödinger equation and to do as much physics as I could without doing that, is that I really believed at that time, in 1941-42, that this back action, this Wheeler-Feynman thing was really a forward step. That's why I was doing everything. I wanted to get the quantum mechanics of that, and that was in the form of a path integral; it had no Hamiltonian.

And also in his thesis, we see Feynman wrestling with these issues, as in the following long quote, where he argues that one should at least keep the notion of an asymptotic, free state in order to interpret the theory:

> It is not unreasonable that it should be impossible to find a quantity like a wave function, which has the property of describing the state of the system at one moment, and from which the state at other moments may be derived. In the more complicated mechanical systems [of action-at-a-distance] the state of motion of a system at a particular time is not enough to determine in a simple manner the way the system will change in time. It is also necessary to know the behavior of the system at other times; information which a wave function is not designed to furnish. An interesting, and at present unresolved, question is whether there exists a quantity analogous to a wave function for these more general systems, and which reduces to the ordinary wave function in the case that the action is the integral of a Lagrangian. That such exists is, of course, not at all necessary. Quantum mechanics can be worked entirely without a wave function, by speaking of matrices and expectation values only. In practice, however, the wave function is a great convenience, and dominates most of our thought in quantum mechanics. For this reason we shall find it especially convenient, in interpreting the physical meaning of the theory, to assume our mechanical system is such that, no matter how complex between the time T_1 and T_2, outside of this range the action is the integral of a Lagrangian. In this way, we may speak of the state of a system at time T_1 and T_2, at least, and represent it by a wave function.

We can thus see, how the two war year programs of eliminating the notion of state from quantum mechanics can both be viewed as directly resulting from the perceived inability of a quantum field theory to address questions of incremental time evolution. We have already seen that Heisenberg's program of using his S matrix as the basis for a new QFT failed: It remained, for the time being, an empty theoretical structure. How did Feynman's least action formalism fare as the foundation of a new QED? What became of the attempt at using it to quantize Wheeler-Feynman electrodynamics? It is to this question that we now turn.

2.4 The Quantization of Action at a Distance Theories

The short answer is: Feynman did not quantize Wheeler-Feynman electrodynamics in his thesis. The first major difficulty was in fact not the action at a distance, but rather the relativistic kinematics of the particles. This was also the problem Wheeler was struggling with [Mehra 1994, 130]. Feynman would return to these questions only after the war, when his struggle with the Dirac equation began, which is recounted in great detail in [Wüthrich 2010]. We will also return to this point. For his thesis, Feynman restricted himself to non-relativistic theories.

Apart from the difficulties of relativistic kinematics, there was a further major, and more general, problem in Feynman's approach to quantizing non-Lagrangian theories. He was, in fact, very unsatisfied with circumventing the problem of the lack of a state described by a wave function by talking only of free, asymptotic states. In the section following the long quotation above, he went on to write (p.49):

> The physical interpretation which is given in the above section, although the only consistent one available, is rather unsatisfactory. This is because the interpretation requires the concept of states representable by a wave function, while we have pointed out that such a representation is in general impossible. We are therefore forced to alter our mechanical problem so that the action has a simple form at large future and past times, so that we may speak of a wave function at these times, at least. [...] We have not defined precisely what is to be done when the action does not become simple at times far from the present.
> One possibility that suggests itself is to devise some sort of limiting process so that the interpretation of the last section could be used, and the limit taken as $T_1 \to -\infty$ and $T_2 \to +\infty$. The author has made several attempts in this direction but they all appear artificial, having mathematical, rather than physical, content.

Feynman thus attempted to construct a formulation of the theory in which there was no more talk of initial and final states at all:

> An alternative possibility is to avoid the mention of wave function altogether, and use, as the fundamental physical concept, the expectation value of a quantity, rather than a transition probability.

This attempt was plagued by difficulties: Feynman could not devise a general method to get only real expectation values for physical quantities. This was especially problematic concerning the expectation value of the energy, where a complex expectation value implied the loss of unitarity (i.e., probabilities did not add up to one). In his Nobel lecture, Feynman stated that he wrote up his thesis in "in one of the short periods during which I imagined I had laid [the difficulty] to rest." But even in his thesis he characterized his approach as "very incomplete and the results tentative." And indeed, in the following years he reached the conclusion that it would not work:

> During the war, I didn't have time to work on these things very extensively, but wandered about on buses and so forth, with little pieces of paper, and struggled to work on it and discovered indeed that there was something wrong, something terribly wrong.

Returning to these questions after the war in earnest, he somewhat grudgingly accepted working with asymptotic free states, as witnessed, e.g., by the following quote from a later paper Feynman [1950]:

> [W]e can imagine the charges to be turned on after [T_1] adiabatically and turned off slowly before [T_2] [...]. Hereafter we shall [...] consider the range of integration of t to be from $-\infty$ to $+\infty$, imagining, if one needs a definition, that the charges vary with time and vanish in the direction of either limit.

While it is not necessary for our story to study in detail Feynman's attempts at eliminating even the asymptotic states, it is important to understand how this affected his approach to the quantization of non-Lagrangian theories. The incompleteness of his quantization program implied that he could not simply take the action for a non-relativistic theory of action at a distance and plug it into a path integral. Instead, he took a more conservative approach.

Recall that Wheeler-Feynman electrodynamics is removed from the classical field theory in two steps, which are related to the two difficulties of QED that Feynman had learned as an undergrad. First, there is the elimination of the field degrees of freedom and their replacement by a half-retarded, half-advanced direct interaction. The resulting theory of particles interacting at a distance is equivalent to the field theory - the only modification is that a certain solution of the field equations has been singled out. The second step is the removal of the electron's self-interaction, which makes the resultant theory inequivalent to the field theory.

Instead of now directly quantizing a non-Lagrangian theory, Feynman only attempted to find a quantum mechanical generalization of the elimination of the field. The resultant quantum theory would then of course not have a Lagrangian and was supposed to be describable only in terms of Feynman's "expectation value" formulation of the path integral for non-Lagrangian theories. But at the same time, he was able to keep a clear relation to a theory formulated in the well-established language of Hamiltonian QM. Expressed positively, as Feynman did in the abstract of his thesis, this meant that "the results serve as a confirmation of the proposed generalization." One can of course also read this, as saying that Feynman did not dare venture too far into unknown territory with the tentative (and soon to be discarded) tools he had at hand.

The non-relativistic toy model for the elimination of the field was the interaction of two particles (coordinates y and z, respectively) interacting via a harmonic oscillator (coordinate x, mass m, frequency ω), described classically by (the oscillator not yet eliminated) the Lagrangian:

$$L = L_y + L_z + \left(\frac{m\dot{x}^2}{2} - \frac{m\omega^2 x^2}{2} \right) + \gamma x \tag{13}$$

where I_y and I_z are arbitrary functionals of $y(t)$ and $z(t)$, respectively, describing the interaction of the particles with the oscillator. This was a natural starting point, since QED could be formulated, and this is how Feynman learned it from Fermi's influential 1932 RMP review, as a set of particles interacting via a continuum of harmonic oscillators, one for each of the modes of the electromagnetic field.

In the classical theory, one can now eliminate the oscillator degree of freedom by solving the Euler-Lagrange equation of motion for the oscillator, and then plugging the chosen solution (which will be a functional of $y(t)$ and $z(t)$ and a function of the boundary conditions imposed on the oscillator) into the equations of motion for the particle. The important fact is that the oscillator equation of motion can be solved independently because the interaction term is linear in x, making the inhomogeneous term in the oscillator equation of motion merely a function of y and z.

The important question is then, whether the new equations of motion for the particles, which are no longer of the Euler-Lagrange form, can still be obtained from the minimization of some new action, which is then of course no longer simply the time integral of a Lagrangian. Feynman could show that this depended on what type of boundary conditions one used to specify the solution of the harmonic oscillator equation of motion, and what kind of parameters would consequently show up in the action-at-a-distance particle equations of motion.

If one specified the initial conditions (position and velocity, i.e., the usual Cauchy boundary conditions) of the oscillator, one ended up with equations of motions for the particles that could not be derived from an action. If one instead specified the position at some initial and another final time (Dirichlet boundary conditions), one did end up with a theory that could be cast into an action. Feynman finally considered imposing conditions on two specific linear combinations R_0 and R_T of initial ($t = 0$) and final ($t = T$) positions and velocities (a special case of Robin boundary conditions):

$$\begin{aligned} R_0 &= \frac{1}{2}\left[x(0)+x(T)\cos\omega T - \dot{x}(T)\frac{\sin\omega T}{\omega}\right] \\ R_T &= \frac{1}{2}\left[x(T)+x(0)\cos\omega T - \dot{x}(0)\frac{\sin\omega T}{\omega}\right] \end{aligned} \tag{14}$$

These boundary could be interpreted in the following way:

> R_T is the mean of the coordinate of the oscillator at time T and what the coordinate would have been at this time if the oscillator had been free and started with its actual initial conditions. Similarly, R_0 is the mean of the initial coordinate and what that coordinate would have had to be, were the oscillator free, to produce the actual final conditions at time T.

They also led to an action-at-a-distance particle action, which depended on the parameters R_0 and R_T. Of particular interest to Feynman was the special case, where both of these parameters are set equal to zero. Given his physical interpretation of the boundary conditions, this choice of parameters can easily be interpreted as the oscillator being in its classical ground state (located at the origin, zero velocity), both for initial and final times. The resulting action for this parameter choice had the special feature that the initial and final times could unproblematically be taken to negative and positive infinity, respectively. The action in this limit

$$\mathscr{A} = \int_{-\infty}^{\infty} \left[L_y + L_z\right] dt + \frac{1}{2m\omega}\int_{-\infty}^{\infty}\int_{-\infty}^{t} \sin\omega(t-s)\gamma(t)\gamma(s)\,ds\,dt \tag{15}$$

where γ is short for $I_y + I_z$, was then also time translation invariant and thus allowed for the definition of a conserved energy, which now of course was a function of the full particle trajectories.

The special significance of this action for Feynman is not immediately apparent upon a cursory reading of his thesis. [Mehra 1994, p. 133] claims that Feynman somehow proved the uniqueness of this choice of boundary conditions, given the constraints of obtaining a time translation invariant action. This is, however, certainly an exaggeration (e.g., Feynman considered neither Neumann boundary conditions, nor more general Robin boundary conditions) and Feynman never makes such a claim. Mehra further identifies the choice of boundary conditions as chosing "a definitely determined solution of the oscillator equation, a symmetric one which included one-half advanced and one-half retarded interaction between the atoms." But this physical interpretation is very unclear: If there is only one oscillator, there is no dispersion relation and consequently neither a group or a phase velocity, which might give a meaning to the notion of advanced or retarded interactions; and again, Feynman makes no such claim. What he did remark, off-handedly, was that

> In electrodynamics it [the action of equation 15] leads to the half advanced plus half retarded interaction used in the action at a distance theory.

Indeed, as Feynman showed in his thesis, one can generalize the procedure outlined above to the case of a large number of oscillators. In particular (and this Feynman did not do explicitly in his thesis), one can generalize to the case of electrodynamics, with one oscillator for each radiation mode of the electromagnetic field. Further generalizing to the case of velocity-dependent interactions (which Feynman had refrained from doing in his thesis (p. 18) "for simplicity only"), one can take the interaction of a particle (described by its position vector $\mathbf{y}$ and possessing a charge q) with the oscillator corresponding to the radiation mode of wave vector $\mathbf{K}$ (frequency $c|\mathbf{K}|$) and polarization vector $\mathbf{e}$ to be given by the usual minimal coupling of electron theory[5]

$$I_y = \sqrt{8\pi} q_y \left(\mathbf{e} \cdot \dot{y}\right) \cos\left(\mathbf{K} \cdot \mathbf{y}\right) \tag{16}$$

After eliminating all the oscillators, with boundary conditions $R_0 = R_T = 0$ for each one of them, the resultant action indeed describes half-advanced, half-retarded electromagnetic interactions, i.e., it is the Fokker action, but with an additional self-energy term. Feynman's above comment and the central role that the action of equation 15 clearly indicate that he was aware of this.

Then why didn't Feynman include such an analysis in his thesis, making the connection between his toy model and Wheeler-Feynman electrodynamics more explicit? There is an additional difficulty in obtaining half-advanced, half-retarded action at a distance through the elimination of the electromagnetic mode oscillators: In addition to the Fokker action (plus self-energy), there are additional boundary terms, which can only be made to vanish by assuming that the interaction is adiabatically turned off in the distant past and future. And as we have seen, Feynman was very hesitant to make such assumptions at the time. This may well explain why he only hinted in passing at the connection between his toy model and the Fokker action.

Restricting himself to the one-oscillator toy model, the next question still was: How was the elimination of the oscillator to be carried over into the quantum theory? The general idea was clear: Given a path integral involving both the particles and the oscillator, one would perform the integration only over the coordinates of the oscillator and arrive at a new expression for the matrix element in question that would now only involve (functional) integration over the coordinates of the particles. Feynman showed how this could be done in general, effectively developing techniques for the functional integration of Gaussian integrals. But what now was the analogue of the classical choice of boundary conditions for the oscillator?

The obvious answer would seem to be setting the initial and final quantum mechanical states of the oscillator. But this obvious answer was not available to Feynman at the time, since he

[5]Note that for each such oscillator there is another one with the cosine replaced by a sine in the interaction term.

was attempting to eliminate the notion of state altogether. The alternative he presented in his thesis is quite involved, but basically boils down to simply choosing some boundary conditions for the oscillator coordinate and its time derivative, in full analogy to the classical theory. The (rather unspectacular) result was then that a given choice of boundary conditions always led to the same action-at-a-distance theory, no matter whether the oscillator was eliminated classically or quantum mechanically. This is where Feynman left things when heading off to Los Alamos.

His work immediately after the war was, as already mentioned, mainly devoted to the Dirac equation. He returned to the question of arriving at a theory of direct particle interaction by eliminating intermediate oscillators when writing his review article on the path integral in 1947. As already discussed, he had by this time abandoned his attempts at removing also the asymptotic states from the theory. Consequently, when presenting the elimination of the oscillator degrees of freedom in his review article, he set the boundary conditions for the quantum oscillator one wants to eliminate by specifying the initial and the final wave function of the oscillator.

Here something interesting happens: The natural quantum generalization of the choice of boundary conditions Feynman had favored in his thesis ($R_0 = R_T = 0$) is of course to take the quantum mechanical ground state as the initial and final state for the oscillator. It turns out, now, that this does *not* lead to the same action as in the classical case, i.e., for electrodynamics to a half-advanced, half-retarded interaction. Instead, in quantum theory, this choice of boundary conditions leads to the usual full retarded interaction.

It is not entirely clear when Feynman became aware of this: The first extant calculations by Feynman on this matter date from around the time of the completion of the review article. But already in 1942, when writing up his thesis, Feynman realized that the technique of eliminating the field/oscillators would have applications in QED proper, independent of all considerations of advanced actions at a distance and self energy elimination.

It was in fact, as Feynman had learned in particular from reading Fermi's introduction to QED, standard procedure to eliminate some components of the electromagnetic field in the quantum theory, namely those corresponding to the longitudinal and time-like modes of the electromagnetic four-potential, i.e., those components which did not correspond to propagating electromagnetic radiation. They could be eliminated without recourse to path integral techniques (which of course were not available at the time), simply by using the gauge freedom of electrodynamics - their elimination in fact was equivalent to a specific choice of gauge, nowadays known as the Coulomb gauge, because the resulting Hamiltonian after the elimination now contains an instantaneous interaction at a distance between the electrons, the well-known Coulomb interaction.

The elimination of the longitudinal and time-like modes meant a huge simplification for calculations in QED, and Feynman hoped that a generalization of this procedure, using his techniques, in which also the transverse, radiation modes of the field were eliminated would lead to even greater simplifications, in particular he hoped that it might shed light on the question of self-energy - Wheeler-Feynman electrodynamics is only mentioned in a footnote. Concerning the elimination of the oscillators in QED, he wrote:

> [T]he oscillators representing longitudinal waves may be eliminated. The result is instantaneous electrostatic interaction. The electrostatic elimination is very in-

> structive as it shows up the difficulty of the self-interaction very distinctly. In fact, it shows up so clearly that there is no ambiguity in deciding what term is incorrect and should be omitted. This entire process is not relativistically invariant, nor is the omitted term. It would seem to be very desirable if the oscillators, representing transverse waves, could also be eliminated. This presents an almost insurmountable problem in the conventional quantum mechanics. [...]
> The present formulation permits the solution of the motion of all the oscillators and their complete elimination from the equations describing the particles. This is easily done.

Feynman's attempts at constructing a new quantum theory of electrodynamics had thus led him instead to a reformulation of QED, one in which states were not eliminated (for the resulting theory was still to be equivalent to the usual formulation with all the oscillators in place), but in which they were very much marginalized (for there were no more states, except for asymptotic free ones, after the oscillators were eliminated). Just like Heisenberg's S matrix, this reformulation would turn out to be extremely powerful in the context of the re-invention of QED in the late 1940s, shaping the reformulation of QFT in a decisive manner.

To be continued

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