Quantum field theory is investigated in the Schrödinger picture without using time-ordered perturbation theory (Feynman diagrams) and without producing singularities. The many-particle Schrödinger equation of quantum electrodynamics is set up and solved numerically for special cases, including pair annihilation and creation. This non-perturbative quantisation method makes it possible to combine quantum field theory and general relativity without divergences. In particular it provides a natural way to quantise noncommutative geometry.

### I. INTRODUCTION

The most precise description of nature currently provided by theoretical physics consists of general relativity and quantum field theory. Perturbative methods based on time-ordered products, in particular Feynman diagrams, have proven extremely successful for studying the Standard Model of quantum field theory. Applying the same methods to general relativity leads to nonrenormalisable divergences.

So far none of the suggested solutions to this problem, notably string theory and loop quantum gravity, has been backed by experiments [1, §2C]. The same holds for ongoing attempts to unify the ingredients of the Standard Model, electroweak interaction and quantum chromodynamics. In particular, in spite of extensive search, there is currently no experimental evidence for supersymmetry.

A different approach is noncommutative geometry [2]. It unifies all fundamental forces of physics by ascribing them to gravity on a non-commutative spacetime with discrete extra dimensions. It does not address the non-renormalisable divergences which arise from applying the established perturbative quantisation methods to gravity. Instead it successfully uses the methods of general relativity to study the foundations of quantum field theory. The main point of criticism of noncommutative geometry is that no quantisation procedure compatible with this framework has been found so far [3].

This work pursues the strategy of noncommutative geometry to apply the tools of general relativity to quantum field theory. Instead of adapting gravity for established quantisation methods, we develop and implement a new, non-perturbative quantisation method, which is compatible with general relativity and naturally fits into noncommutative geometry. Working in the Schrödinger picture, we extend the methods of mathematical physics from the one-particle Dirac equation [4, §§28.4–28.5] to many-particle quantum electrodynamics. To solve the resulting hyperbolic partial differential equation numerically we develop a new explicit algorithm with adaptive stepsize.

Methods of this type are commonly applied to classical fields. This is the first time a method which is compatible with general relativity has been successfully applied to simulate pair annihilation and creation in quantum fields.

### II. QUANTUM ELECTRODYNAMICS – THE SCHROEDINGER PICTURE

We start from the well-known Lagrangian density of quantum electrodynamics,

\[
\mathcal{L} = \bar{\psi}(i\hbar c\gamma^\mu \partial_\mu - q^\mu A_\mu - mc^2)\psi - \frac{1}{4} F_{\mu\nu} F^{\mu\nu}. \tag{1}
\]

By keeping \(c, \hbar\) and the coupling constant \(q\) (charge) as variables instead of setting them to 1 we leave the door open for studying the limits \(c \to \infty\) and \(\hbar \to 0\).

We derive the Hamiltonian density,

\[
\mathcal{H} = \bar{\psi}(mc^2 - i\hbar c \gamma^j \partial_j)\psi + \frac{1}{4} F_{\mu\nu} F^{\mu\nu} - \bar{\psi} q \gamma^\mu A_\mu \psi, \tag{2}
\]

and substitute the time-independent field operators

\[
\hat{\psi}(x) = \int d^3 p \sum_{\sigma = 0}^3 \psi_{p,\sigma}\gamma_{p,\sigma} e^{-\frac{i}{\hbar} px}, \tag{3}
\]

\[
\hat{\bar{\psi}}(x) = \int d^3 p \sum_{\sigma = 0}^3 \bar{c}_{p,\sigma}\psi_{p,\sigma} e^{\frac{i}{\hbar} px}, \tag{4}
\]

\[
\hat{A}_\mu(x) = \int d^3 k \sqrt{\frac{\hbar c}{2\pi}} \left( a_{k,\mu} e^{ikx} + a_{k,\mu}^* e^{-ikx} \right) \tag{5}
\]

for the wave functions \(\psi, \bar{\psi}\) (fermions), and \(A_\mu\) (photons). For \(\sigma \in \{0, 1, 2, 3\}\), \(\psi_{p,\sigma}\) denotes the normalised amplitude of the spinor-valued momentum eigenstate with momentum \(p\), with positive energy for \(\sigma \in \{0, 1\}\) or negative energy for \(\sigma \in \{2, 3\}\). \(\bar{c}_{p,\sigma} = \gamma^\sigma \psi_{p,\sigma}^*\) denotes the Dirac adjoint of \(\psi_{p,\sigma}\).

The fermionic ladder operators \(c_{p,\sigma}\) and \(c_{p,\sigma}^+\) are kept generic for now and will be reinterpreted later to separate particles and anti-particles,

\[
c_{p,\sigma} = b_{p,\sigma}, \quad c_{p,\sigma}^+ = b_{p,\sigma}^+ \quad \text{for } \sigma \in \{0, 1\}, \tag{6}
\]

\[
c_{p,\sigma} = d_{p,\sigma}, \quad c_{p,\sigma}^+ = d_{p,\sigma}^+ \quad \text{for } \sigma \in \{2, 3\}. \tag{7}
\]

\(a_{k,\mu}\) and \(a_{k,\mu}^*\) denote the photonic ladder operators for the \(\mu\)th component of a plane wave of the electromagnetic four-potential.

Following the customary path of quantum electrodynamics, we separate \(e^{-\frac{i}{\hbar} px}\) from the momentum eigenstates, recombine them, carry out the integrals over \(x\) and \(p\), and obtain the Hamiltonian

\[
H = \int d^3 x \mathcal{H}(x) = H_\psi + H_A + H_J \tag{8}
\]
which consists of the Hamiltonian of free fermions

$$H_\psi = \int d^3 p \sum_{\sigma=0}^3 \epsilon_{p,\sigma}^+ \bar{\psi}_{p,\sigma}(mc^2 - i\hbar c \gamma^j \partial_j) \psi_{p,\sigma} \epsilon_{p,\sigma},$$

(9)

the Hamiltonian of free photons,

$$H_A = \int d^3 k \sum_{\mu=0}^3 \frac{1}{2} \hbar \omega_k (a_{k,\mu}^+ a_{k,\mu} + a_{k,\mu} a_{k,\mu}^+),$$

(10)

where $\omega_k = c|k|$, and the interaction Hamiltonian

$$H_I = -qc \int d^3 p \int d^3 k \sum_{\mu=0}^3 \sqrt{\frac{\hbar c^2}{2\omega_k}} (a_{k,\mu} + a_{k,\mu}^+) \epsilon_{p,\sigma}^+ \bar{\psi}_{p,\sigma} \gamma^\mu \psi_{p,\sigma},$$

(11)

In the free Hamiltonians $H_\psi$ and $H_A$ the ladder operators combine to particle number operators and do not cause any serious trouble. The non-perturbative treatment of the interaction Hamiltonian $H_I$ while taking account of fermions and anti-fermions is nontrivial and will be the main topic of this paper.

A. Dynamics of the Fermions

Our Schrödinger equation

$$i\hbar \frac{\partial}{\partial t} \psi(t) = H \psi(t),$$

(12)

has the formal solution

$$\psi(t + \Delta t) = \exp \left( -\frac{i}{\hbar} \int_0^{\Delta t} H dt' \right) \psi(t),$$

(13)

where $\psi(t)$ denotes the combined wave function of the fermions and the photons.

Instead of expanding the exponential into a power series, we proceed by writing the operator inside the exponential in its eigenbasis, so we can carry out the exponential without approximation.

Other approximations cannot be avoided. Even considering $H_J$ as a linear operator is an approximation because of the coupling between the fermions and the photons. To get it manageable we make the time interval $\Delta t$ small, so we can calculate the time development of the fermions under the influence of the stationary photons, and vice versa.

The same approximation allows us to replace the integral by a multiplication and to neglect the non-commutativity of the ingredients of $H$,

$$e^{-\frac{i}{\hbar} H \Delta t} = e^{-\frac{i}{\hbar} H_\psi \Delta t} e^{-\frac{i}{\hbar} H_A \Delta t} e^{-\frac{i}{\hbar} H_I \Delta t} + O(\Delta t^2).$$

(14)

This approximation can be improved to higher orders of $\Delta t$; see [5] for details.

$H_c$ is diagonal in momentum representation. Together with the $\gamma^0$ from the Dirac adjoint $\psi_{p,\sigma}$ we write it as a matrix over spinor space for each momentum $p$,

$$H_\psi(p) := \gamma^0 mc^2 - \sum_{j=1}^3 c_j \gamma^j p_j.$$

(15)

When we store the fermionic wave functions in momentum representation and decompose them, at each momentum $p$, into eigenstates of $H_\psi(p)$, we can apply $e^{-\frac{i}{\hbar} H_c \Delta t}$ to the wave functions without further approximation.

Essentially the same is possible for $H_I$ in position representation, but it requires some preparation.

As the first step, we apply a reverse Fourier transform to $H_I$ from momentum to position representation. This turns the double integral over $p$ and $k$, a convolution, into a single integral over $x$,

$$H_I = -(2\pi)^\frac{3}{2} q c \int d^3 p \sum_{\sigma=0}^3 \sum_{\sigma'=0}^3 \epsilon_{p,\sigma}^+ \bar{\psi}_{p,\sigma} \gamma^\mu \epsilon_{p,\sigma'} \bar{\psi}_{p,\sigma'} \psi_{x,\sigma} (c_{x,\sigma} + a_{x,\sigma}^+),$$

(16)

where $F$ denotes the Fourier transformation, and

$$a_{x,\mu} = F^{-1} \left( \sqrt{\frac{\hbar c^2}{2\omega_k}} a_{k,\mu} \right)(x),$$

(17)

$$\psi_{x,\sigma} c_{x,\sigma} = F^{-1} \left( \psi_{-p,\sigma} c_{-p,\sigma} \right)(x).$$

(18)

The actual interaction is now diagonal in position representation. Thus it makes sense to speak of the interaction at a specific position $x$, preserving causality.

While we deal with the fermions, we replace all photonic ladder operators $a_{k,\mu}, a_{k,\mu}^+$ by their expectation values $A_{\mu}(k), A_{\mu}^+(k)$ in the current state of the system, the electromagnetic field. As will be shown later, this approximation is surprisingly accurate.

Although we have switched from momentum to position representation, the indices $\sigma$ and $\sigma'$ of the fermionic ladder operators $c_{x,\sigma}^+$ and $a_{x,\sigma}^+$ still refer to momentum eigenstates. It is tempting to carry out the sums over $\sigma$ and $\sigma'$ to make the ladder operators together with the momentum eigenstates sum up to a unity operator. We do not do that because we will still need them later to distinguish between particles ($\sigma \in \{0,1\}$) and anti-particles ($\sigma \in \{2,3\}$).

At a given position $x$ the electromagnetic field and the Dirac matrices form a Hermitian matrix $A(x)$ in spinor space which has the same structure as the momentum operator, again together with the $\gamma^0$ from $\psi_{x,\sigma'}$,

$$A(x) := \sum_{\mu=0}^3 \left( A_{\mu}(x) + A_{\mu}^+(x) \right) \gamma^0 \gamma^\mu.$$

(19)

We decompose the fermionic wave function – in a given momentum eigenstate $\sigma$, but in position representation
and at a given position \( x \) into the eigenstates of \( A(x) \), so we can directly apply the exponential.

The result is no longer a momentum eigenstate, but we can decompose it into momentum eigenstates \( \sigma' \) after we have Fourier transformed the wave functions back to momentum representation.

### B. Fermions and Anti-Fermions

It is the recomposition into particle and anti-particle states, which implements pair annihilation and pair creation. To make this obvious, we revisit the interaction Hamiltonian \( H_J \) in momentum representation and write it as

\[
H_J = -\frac{q}{\hbar} \int d^3p' \sum_{\sigma' = 0}^3 \int d^3p \sum_{\sigma = 0}^3 c_{p',\sigma}^\dagger \bar{\psi}_{p',\sigma'} \psi(p' - p) c_{p,\sigma}.
\]

with the interaction matrix

\[
A(\hbar k) = \sum_{\mu=0}^3 \sqrt{\frac{\hbar c}{2m}} (a_{k,\mu} + a_{-k,\mu})^\dagger \gamma^\mu.
\]

\( H_J \) contains the operator \( c_{p',\sigma}^\dagger c_{p,\sigma} \), which maps the momentum eigenstate \( \psi_{p,\sigma} \) to the momentum eigenstate \( \psi_{p',\sigma'} \). It also contains \( c_{p,\sigma}^\dagger c_{p',\sigma'} \), which does the opposite. Thus the restriction of \( H_J \) to the two-state subspace of the momentum eigenstates \( \psi_{p,\sigma} \) and \( \psi_{p',\sigma'} \) can be written using

\[
c_{p',\sigma'} c_{p,\sigma} + c_{p,\sigma}^\dagger c_{p',\sigma'} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}.
\]

When we denote the two components of our wave function in this subspace by

\[
\psi_0(t) := (\psi_{p,\sigma} | \Psi(t) \rangle), \quad \psi_1(t) := (\psi_{p',\sigma'} | \Psi(t) \rangle),
\]

the interaction part of a time step of length \( \Delta t \) in the solution of our Schrödinger equation in this subspace reads, up to \( \mathcal{O}(\Delta t^2) \),

\[
\begin{pmatrix} \psi_1(t + \Delta t) \\ \psi_0(t + \Delta t) \end{pmatrix} = e^{-\frac{i}{\hbar} H_J \Delta t} \begin{pmatrix} \psi_1(t) \\ \psi_0(t) \end{pmatrix} = \exp(iC \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}) \begin{pmatrix} \psi_1(t) \\ \psi_0(t) \end{pmatrix} = \begin{pmatrix} \cos C \psi_1(t) + i \sin C \psi_0(t) \\ \cos C \psi_0(t) + i \sin C \psi_1(t) \end{pmatrix},
\]

where

\[
C := -\frac{q}{\hbar} \Delta t A(p' - p).
\]

So the interaction manifests as a complex “rotation” between two fermionic eigenstates.

In the case where both fermionic eigenstates \( \psi_{p,\sigma} \) and \( \psi_{p',\sigma'} \) denote (anti-) particles, eq. 25 describes the transition between two states of the (anti-) particle with different momenta and different spins resulting from emission or absorption of photons with momentum \( h \bar{p} = p' - p \).

In the other case one eigenstate belongs to a particle and the other one to an anti-particle. Then we must reinterpret the ladder operators according to Feynman-Stückelberg.

Let \( \psi_{p,\sigma} \) describe a particle and \( \psi_{p',\sigma'} \) an anti-particle. Then \( c_{p,\sigma} = b_{p,\sigma} \) remains an annihilation operator for a particle, but the creation operator becomes another annihilation operator for a spacetime-mirrored anti-particle, \( c_{p',\sigma'}^\dagger = d_{-p',\sigma'} \). Likewise, \( c_{p,\sigma}^\dagger = b_{-p,\sigma}^\dagger \) and \( c_{p',\sigma'} = d_{-p',\sigma'}^\dagger \). Their combination \( c_{p',\sigma'}^\dagger c_{p,\sigma} = d_{-p',\sigma'} b_{-p,\sigma} \) maps the two-particle state to the vacuum state.

Now we reverse the roles of \( p, \sigma \) and \( p', \sigma' \). Then \( \psi_{p,\sigma} \) describes an anti-particle and \( \psi_{p',\sigma'} \) a particle, and the combined operator \( c_{p',\sigma'}^\dagger c_{p,\sigma} = b_{-p',\sigma'}^\dagger d_{p,\sigma} \) maps the vacuum state to the two-particle state.

Again \( H_J \) contains both combinations. We write their sum as

\[
d_{-p',\sigma'} b_{p,\sigma} + b_{-p,\sigma}^\dagger d_{-p',\sigma'}^\dagger = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}.
\]

Eq. 25 applies without change, but now it rotates between the vacuum state and the two-particle state. Depending on which one of both states is occupied, this case describes both pair annihilation and pair creation.

When we perform calculations and simulations with these wave functions, we represent the anti-particles as “Dirac holes”, i.e. as \( CPT \)-reversed vacuum wave functions. There are several methods to implement this. Special care must be taken when decomposing and recombining two fermionic wave functions in momentum representation, one of which is \( CPT \)-reversed. Again see \[5\] for details.

As a side note, this reaffirms that the “Dirac sea” approach, which is also used in noncommutative geometry \[6, \S 4\], is equivalent to the Feynman-Stückelberg interpretation.

In summary, we can compute the effect of the time development operator \( e^{-\frac{i}{\hbar} H_J \Delta t} \) on the fermions as follows.

- The fermions are stored as two spinor-valued wave functions. One represents the particles. The other one stores the anti-particles as Dirac holes.
- At each momentum \( p \), we decompose the fermionic wave functions into eigenstates of \( H\psi(p) \) and apply \( e^{-\frac{i}{\hbar} H\psi(p) \Delta t} \) to them, taking into account that the wave function of the anti-particles is \( CPT \)-reversed.
- We switch from momentum to position representation by applying reverse Fourier transforms to all wave functions.
- At each position \( x \), we decompose the fermionic wave functions into eigenstates of \( A(x) \) and apply \( e^{-\frac{i}{\hbar} H_J \Delta t} \).
We switch back to momentum representation by applying Fourier transforms to all wave functions.

We decompose the resulting fermionic wave functions into momentum eigenstates and recombine them into wave functions of particles and of antiparticles.

By iterating this procedure we can calculate the time development of the fermions under the influence of the photons.

C. Dynamics of the Photons

The time development operator for the interaction of the photons can be written as

\[ e^{-i \hbar H_J \Delta t} = \exp \left( \int d^3k \sum_{\mu=0}^{3} \alpha_{\mu}(k) a_{k,\mu}^+ - \alpha_{\mu}^*(k) a_{k,\mu} \right), \]  

(28)

where

\[ \alpha_{\mu}(k) = \frac{i\hbar c}{k} \Delta t \int d^3 p \sum_{\sigma=0}^{3} \sum_{\sigma'=0}^{3} \bar{\psi}_{p+hk,\sigma'} \gamma^\mu \psi_{p,\sigma} c_{p+hk,\sigma'}^+ c_{p,\sigma}. \]  

(29)

This is a displacement operator for coherent states in momentum representation, which implies that the time development operator for photons under the influence of fermions maps a coherent state to another coherent state. Since the same holds for the free time development of photons this shows that photonic coherent states always remain coherent in quantum electrodynamics.

The integral over \( p \) is a convolution which can be calculated using Fourier transforms from momentum to position representation and back. Thus the actual interaction takes place in position representation, where it acts locally rather than over a distance, and causality is maintained.

A coherent state with parameter \( \alpha_{k,\mu} \) is an eigenstate of the matching annihilation operator \( a_{k,\mu} \). Thus our approximation in subsection II A, where we substituted all photonic ladder operators with their expectation values in the current state of the photons, is in fact exact, provided that the initial state of the photons is a coherent state itself. This holds, for instance, for the vacuum state.

The free development of a coherent state is well-known. Together with eq. 28 this allows us to simulate the full dynamics of the photons, storing them as a field of coherent states.

III. NUMERICAL RESULTS

As we have seen above, the “natural” way to describe a many-particle system of fermions and photons in the Schrödinger picture consists of two spinor-valued wave functions for the fermions and the anti-fermions, plus a field of coherent states for the photons. To simulate the time development of such a system in a computer we store all three wave functions point-wise.

Due to limitations of computer memory and calculation performance we restrict ourselves to two spatial dimensions.

By applying the steps described above iteratively we can simulate the time development of an initial state. This method is similar to the explicit Euler method of first order in \( \Delta t \). It can be improved to higher orders of \( \Delta t \), and we can implement time-step control. See [5] for details.

The numeric computation of the Fourier transforms
on a discretised space [7] induces periodic boundary conditions. To avoid interference of the outgoing photonic wave function with itself we can either make the spatial window so big that the wave function cannot reach the boundary, or absorb it numerically before it does.

We do not simulate the electrostatic fields generated by the fermions because they would make the wave packets dissolve out of numerical visibility before they collide. We suppose that this problem can be solved by increasing the spatial window of the simulation, which would require more computing resources.

To simulate pair annihilation, we prepare wave functions of electrons and positrons as Gaussian wave packets as shown in fig. 1. Their mean positions are separated; their mean momenta are chosen such that they will collide.

Figure 2 shows the state of the simulation after several iterations at $t \approx 0.436$ as. The wave packets of the electrons and positrons have collided and already annihilated parts of each other, generating arc-shaped photonic wave functions.

Figure 3 shows the outgoing wave functions after the collision, at $t \approx 0.579$ as. The norms of the fermionic wave functions have shrunk significantly, leaving behind an outgoing photonic wave function.

Figure 4 shows the time development of the norm of the wave functions. During the pair annihilation the norm of the fermionic wave functions shrinks to less than one quarter of its initial value, which means that the probability for annihilation is over 75% in this scenario. The norm of the photonic wave function grows. The increase of the norm of the fermions after $t \gtrsim 0.5$ as and its small oscillations for $t \lesssim 0.4$ as are due to pair creation. The decrease of the norm of the photons after $t \gtrsim 0.6$ as is due to their absorption at the border of the spatial window of the simulation.
Figure 7. Pair creation: outgoing wave functions, \( t \approx 0.270 \text{ as} \). The outgoing photons are being absorbed at the border of the spatial window of the simulation, leaving behind wave packets of electrons and positrons with small momenta.

Figure 8. Pair creation: norm of the wave functions, scaled by a factor of 5 for the fermions.

To simulate pair creation, we prepare wave functions of two colliding photonic wave packets, plus wave functions of electrons and positrons with zero momentum and negligible norm in the centre. (If we initialised the fermionic wave functions to exact vacuum states, they would remain in that state even if the vacuum state becomes unstable.) Figure 5 visualises this initial state.

The photonic wave packets propagate and get arc-shaped. Where they overlap they leave behind regions where the norm of the fermionic wave functions got increased, see fig. 6 and 7. Figure 8 shows the norm of the wave functions in the case of pair creation. The oscillations of the fermionic wave functions between \( t \approx 0.13 \text{ as} \) and \( t \approx 0.23 \text{ as} \) are due to interference between the two photonic wave packets. Their slight decrease after \( t \gtrsim 0.2 \text{ as} \) is due to annihilation of the newly created pairs. The asymmetry is due to limited numerical precision.

These simulations of pair annihilation and creation are qualitatively correct. In contrast to the well-established perturbative methods they were simulated in a framework whose extension to general relativity is straightforward, but was not thought to be suitable for studying quantum field theory so far.

IV. CONCLUSIONS AND OUTLOOK

The incompatibility between general relativity and quantum field theory consists of nonrenormalisable divergences, which arise from applying time-ordered perturbation theory to gravity.

The approach developed in this paper does the opposite. It applies the main tool of general relativity, solving a partial differential equation, to quantum electrodynamics, the simplest case of quantum field theory. It successfully simulates effects of second quantisation, pair annihilation and creation, without using time-ordered perturbation theory and without producing singularities.

The extension of this method from quantum electrodynamics to the full Standard Model might require significantly more computational power, depending on the transferability of the concept of coherent states from the photons to the other bosons. To include general relativity we have to apply the spin connection to incorporate curvature of spacetime, and we have to use the many-particle wave functions as sources for the Einstein field equations. All this is expected to be laborious, but straightforward.

In conclusion we have developed a new quantisation method which is compatible with gravity and with noncommutative geometry.

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