Quantum field theory in the Schrödinger picture

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The many-particle Schrödinger equation of quantum electrodynamics is set up and solved numerically, using a generalised version of a method from quantum chaos. The results for pair annihilation and creation are qualitatively correct. This is an alternative method for second quantisation, which works in the Schrödinger picture, without using time-ordered perturbation theory (Feynman diagrams). It is thus, by construction, compatible with general relativity and with noncommutative geometry via the spin connection.

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.

The most well-known approaches to overcome this problem are string theory [1] and loop quantum gravity [2]. To date there is, however, no experimental evidence for either of these theories [3, § 2C]. Both approaches have in common that they apply established quantisation methods, path integrals or canonical quantisation, to gravity, predicting quantum effects of spacetime itself such as a granularity at the Planck scale. In both theories it is still an open problem how to recover general relativity.

Another approach is to treat gravity as a classical field together with unmodified quantum field theory. These semiclassical approaches predict quantum phenomena which include gravity, such as Hawking radiation [4] and effects of gravity on the quantum mechanics of macroscopic objects, which might be in range of experimental tests, soon [5].

A promising alternative approach is to change the prescription for second quantisation in such a way that it “interpolates” between perturbatively quantised general relativity at low energies and gravity as a classical field at high energies [6].

A very different approach is noncommutative geometry [7–12]. 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 nonrenormalisable 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 [11]. (Another problem concerning the predicted mass of the Higgs boson has been cleared up [12].)

In this work we develop a non-perturbative method to quantise fermionic and bosonic fields in such a way that they remain compatible with general relativity and with noncommutative geometry via the spin connection.

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

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

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,

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

and substitute the time-independent field operators

$$\bar{\psi}(x) = \int d^3p \sum_{\sigma = 0}^3 \psi_{p,\sigma} c_{p,\sigma} e^{-\frac{\gamma}{\hbar} px},$$

$$\psi(x) = \int d^3p \sum_{\sigma = 0}^3 \bar{c}_{p,\sigma} \bar{\psi}_{p,\sigma} e^{\frac{\gamma}{\hbar} px},$$

$$\hat{A}_\mu(x) = \int d^3k \sqrt{\frac{\hbar c^2}{2\pi^3}} (a_{k,\mu} e^{ikx} + a^+_{k,\mu} e^{-ikx})$$

for the wave functions $\bar{\psi}$, $\psi$ (fermions), and $A_\mu$ (photons).

For $\sigma \in \{0, 1\}$, the normalised amplitude vectors $\psi_{p,\sigma}$ and their Dirac adjoints $\psi_{p,\sigma}^*$ describe eigenstates with positive energy (particles). For $\sigma \in \{2, 3\}$
they describe eigenstates with negative energy (anti-particles).

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,

$$c_{p,\sigma} = b_{p,\sigma}, \quad c_{p,\sigma}^+ = b_{p,\sigma}^\dagger \quad \text{for } \sigma \in \{0, 1\}, \quad (6)$$

$$c_{p,\sigma} = d_{-p,\sigma}^+, \quad c_{p,\sigma}^+ = d_{-p,\sigma} \quad \text{for } \sigma \in \{2, 3\}. \quad (7)$$

The photonic ladder operators $a_{k,\mu}$ and $a_{k,\mu}^+$ correspond to the $\mu$th component of a plane wave of the electromagnetic four-potential with wave vector $k$.

Following the customary path of quantum electrodynamics, we separate $e^{-\pi p x}$ from the momentum eigenstates, recombine them, carry out the integrals over $x$ and $p'$, and obtain the Hamiltonian

$$H = \int d^3x \mathcal{H}(x) = H_\psi + H_A + H_J \quad (8)$$

which consists of the Hamiltonian of free fermions

$$H_\psi = \int d^3p \sum_{\sigma=0}^3 c_{p,\sigma}^+ \bar{\psi}_{p,\sigma} (mc^2 - i \hbar c \gamma^j \partial_j) \psi_{p,\sigma} c_{p,\sigma}, \quad (9)$$

the Hamiltonian of free photons,

$$H_A = \int d^3k \sum_{\mu=0}^3 \frac{1}{2} \hbar \omega_k (a_{k,\mu}^+ a_{k,\mu} + a_{k,\mu} a_{k,\mu}^+), \quad (10)$$

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

$$H_J = -qc \int d^3p \int d^3k \sum_{\mu=0}^3 \sqrt{\frac{\hbar^2 c}{2\omega_k}} (a_{k,\mu} + a_{-k,\mu}^+) \sum_{\sigma=0}^3 \sum_{\sigma'=0}^3 c_{p-hk,\sigma'}^+ \bar{\psi}_{p-hk,\sigma'} \gamma^\mu c_{p,\sigma} \psi_{p,\sigma}. \quad (11)$$

In the free Hamiltonians $H_\psi$ and $H_A$ the ladder operators combine to particle number operators, which are diagonal in momentum representation and do not cause any serious troubles. The non-perturbative treatment of the interaction Hamiltonian $H_J$ 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

$$i \hbar \frac{\partial}{\partial t} \Psi(t) = H \Psi(t) \quad (12)$$

has the formal solution

$$\Psi(t + \Delta t) = \exp \left( -\frac{i}{\hbar} \int_t^{t + \Delta t} H dt' \right) \Psi(t), \quad (13)$$

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

In momentum representation, the free Hamiltonians $H_\psi$ and $H_A$ can be described by diagonal matrices. The interaction Hamiltonian $H_J$ contains a coupling between the fermions and the photons, so we can treat it as a linear operator only in the approximation of small time intervals $\Delta t$. In other words, we calculate the time development of the fermions under the influence of the stationary photons, and vice versa. Then the double integral of $H_J$ makes it a fully-occupied matrix in momentum representation.

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. With a fully-occupied matrix such as $H_J$ this is only in reach of current computers when the total number of basis states involved does not exceed a few thousands. In the field of quantum chaos, this has successfully been applied to bound systems whose Hilbert space is finite-dimensional, for example the kicked top [14, 16–18]. When we want to simulate systems which correspond to experiments in quantum field theory, in particular scattering systems, we need to consider a larger number of eigenstates.

In the following we generalise a method used in the field of quantum chaos for non-relativistic single-particle scattering systems [15] to quantum field theory. The approximation of small time intervals $\Delta t$ allows us to replace the integral by a multiplication and to neglect the non-commutativity of the ingredients of $H$,

$$e^{-\frac{i}{\hbar} H \Delta t} = e^{-\frac{i}{\hbar} H_\psi \Delta t} e^{-\frac{i}{\hbar} H_A \Delta t} e^{-\frac{i}{\hbar} H_J \Delta t} + O(\Delta t^2). \quad (14)$$

This approximation can be improved to higher orders of $\Delta t$; see [19] for details.

The Hamiltonian $H_\psi$ of free fermions is diagonal in momentum representation. Together with the $\gamma^\mu$ from the Dirac adjoint $\bar{\psi}_{p,\sigma}$ we write it as a matrix over spinor space for each momentum $p$,

$$H_\psi(p) := \gamma^0 mc^2 - \sum_{j=1}^3 c \gamma^0 \gamma^j p_j. \quad (15)$$

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 $e^{-\frac{i}{\hbar} H_\psi \Delta t}$ to the wave functions without further approximation.

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

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

$$H_J = -(2\pi)^3 q c \int d^3p \sum_{\sigma'=0}^3 \sum_{\sigma=0}^3 \sum_{\mu=0}^3 c_{p,\sigma'}^+ \bar{\psi}_{p,\sigma'} \gamma^\mu (a_{x,\mu} + a_{x,\mu}^+) \psi_{x,\sigma} \left( c_{x,\sigma} \right)(p), \quad (16)$$
where $\mathcal{F}$ denotes the Fourier transformation, and
\[
a_{x,\mu} = \mathcal{F}^{-1}\left(\sqrt{\frac{\hbar^2}{2\omega_k}} a_{k,\mu}\right)(x),
\]
\[
\psi_{x,\sigma} c_{x,\sigma} = \mathcal{F}^{-1}(\psi_{-p,\sigma} c_{-p,\sigma})(x).
\]

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 $a_{k,\mu}, a_{k,\mu}^\dagger$ by their expectation values $A_k(k), A_k^\dagger(k)$ 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 $c_{x,\sigma}'$, 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 $\tilde{\psi}_{x,\sigma'}$,
\[
A(x) := \sum_{\mu=0}^{3} \left(A_{\mu}(x) + A_{\mu}'(x)\right) \gamma^0 \gamma^\mu.
\]

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
\[
H_J = -qc \int d3p' \sum_{\sigma'=0}^{3} \int d3p \sum_{\sigma=0}^{3} c_{p',\sigma'}^+ \tilde{\psi}_{p',\sigma'} A(p' - p) \psi_{p,\sigma} c_{p,\sigma}
\]
with the interaction matrix
\[
A(hk) = \sum_{\mu=0}^{3} \sqrt{\frac{\hbar^2}{2\omega_k}} (a_{k,\mu} + a_{k,\mu}^\dagger) \gamma^\mu.
\]

The interaction Hamiltonian $H_J$ contains the operator $c_{p',\sigma'}^+ c_{p,\sigma}$, which maps the momentum eigenstate $\psi_{p,\sigma}$ to the momentum eigenstate $\psi_{p',\sigma'}$. It also contains $c_{p,\sigma}'^+ c_{p,\sigma}'$, 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
\[
c_{p,\sigma}'^+ c_{p,\sigma} + c_{p,\sigma}'^+ c_{p,\sigma}' = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}.
\]

When we denote the two components of our wave function in this subspace by
\[
\psi_0(t) := \langle \psi_{p,\sigma} | \Psi(t) \rangle,
\]
\[
\psi_1(t) := \langle \psi_{p',\sigma'} | \Psi(t) \rangle,
\]
the interaction part of a time step of length $\Delta t$ in the solution of our Schrödinger equation in this subspace reads, up to $\mathcal{O}(\Delta t^2)$,
\[
\begin{pmatrix} \psi_1(t + \Delta t) \\ \psi_0(t + \Delta t) \end{pmatrix} = e^{-\frac{\Delta t}{\hbar} H_J} \begin{pmatrix} \psi_1(t) \\ \psi_0(t) \end{pmatrix} = \exp\left(iH_J \Delta t \right) \begin{pmatrix} \psi_1(t) \\ \psi_0(t) \end{pmatrix} = \begin{pmatrix} \cos C \psi_1(t) + i \sin C \psi_0(t) \\ \cos C \psi_0(t) + i \sin C \psi_1(t) \end{pmatrix}.
\]
where
\[
C := -\frac{\hbar}{2} \Delta t A(p' - p).
\]

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 $\hbar k = p' - p$.

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, $c_{p',\sigma} = d_{-p',\sigma'}$. Likewise, $c_{p,\sigma}' = b_{p,\sigma}'$ and $c_{p',\sigma}' = d_{-p',\sigma'}$. Their combination $c_{p,\sigma}' c_{p,\sigma} = d_{-p,\sigma'} b_{p,\sigma}$ 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 $c_{p,\sigma}' c_{p,\sigma} = b_{p,\sigma}' d_{-p,\sigma}$ maps the vacuum state to the two-particle state.

Again $H_J$ contains both combinations. We write their sum as
\[
d_{-p',\sigma'} b_{p,\sigma} + b_{p,\sigma}' d_{-p',\sigma'} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}.
\]

Equation (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 [19] for details.

As a side note, this reaffirms that the “Dirac sea” approach, which is also used in noncommutative geometry [10], is equivalent to the Feynman-Dirac-Stickelberg interpretation.

In summary, we can compute the effect of the time development operator $e^{-\frac{i}{\hbar}Ht}$ 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 $H_p(p)$ and apply the free time evolution operator $e^{-\frac{i}{\hbar}H_p(p)t}$ 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 $H_x(x)$ and apply the the time evolution operator $e^{-\frac{i}{\hbar}H_x(x)t}$ to them, taking into account that the wave function of the anti-particles is CPT-reversed.
- 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 anti-particles.

By iterating this procedure we can calculate the time development of the fermions under the influence of the photons. As mentioned above, this first-order method can be generalised to higher orders of $\Delta t$.

\section{C. Dynamics of the Photons}

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

$$e^{-\frac{i}{\hbar}H_J\Delta t} = \exp\left(\int d^3k \sum_{\mu=0}^3 \bar{a}_{\mu}(k) a_{\mu,\mu} - a_{\mu}^*(k) a_{\mu,\mu}\right),$$

where

$$a_{\mu}(k) = \frac{i}{\hbar} \gamma^\mu \psi_{\mu,\sigma} e^{i k \cdot x}$$

\section{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 [19] for details.
The numeric computation of the Fourier transforms on a discretised space [20] 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.

In the following simulations we visualise the wave functions of the fermions and anti-fermions (spinors) and of the photons (coherent states, four-vectors) using the colour scheme depicted in Fig. 1.

To simulate pair annihilation, we prepare wave functions of fermions and anti-fermions as Gaussian wave packets as shown in Fig. 2. Their mean positions are separated; their mean momenta are chosen such that they will collide.

The simulation works with dimensionless numerical parameters for $\hbar$, $c$, and the fermion masses and charges. When we specialise for electrons and positrons, the time unit is 0.19 attoseconds, and the space unit corresponds to a distance of about 1.16 Ångström between the centres of the two wave packets in the initial state. (See [19] for further details.)

Figure 3 shows the state of the simulation after several iterations. The wave packets of the fermions and anti-fermions have collided and already annihilated parts of each other, generating arc-shaped photonic wave functions.

Figure 4 shows the outgoing wave functions after the collision. The norms of the fermionic wave functions have
shrunken significantly, leaving behind an outgoing photonic wave function.

Figure 5 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 $t \gtrsim 2.7$ and its small oscillations for $t \lesssim 2$ are due to pair creation. The decrease of the norm of the photons after $t > \sim 3.2$ is due to their absorption at the border of the spatial window of the simulation.

To simulate pair creation, we prepare wave functions of two colliding photonic wave packets, plus wave functions of fermions and anti-fermions 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.) In the visualisation we use the same colour scheme, but with a different scale, see Fig. 6.

Figure 7 visualises the initial state. In this simulation the time unit is $0.13$ attoseconds, and the space unit corresponds to a distance of about $0.77$ Ångström between the centres of the two wave packets in the 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. 8 and 9. Figure 10 shows the norm of the wave functions in the case of pair creation. The oscillations of the fermionic wave functions between $t \approx 0.8$ and $t \approx 1.6$ are due to interference between the two photonic wave packets. The slight decrease of the fermionic wave functions after $t > \sim 1.6$ 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 an alternative method for second quantisation, which is compatible with gravity and with noncommutative geometry.

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