A Computer Model of Quantum Field Theory

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Abstract—This paper describes a computer model of Quantum Field Theory (QFT), referred to in this paper as QTModel. After specifying the initial configuration for a QFT process (e.g. scattering) the model generates the possible applicable processes in terms of Feynman diagrams, the equations for the scattering matrix, and evaluates probability amplitudes for the scattering matrix and cross sections. The computations of probability amplitudes are performed numerically. The equations generated by QTModel are provided for demonstration purposes only. They are not directly used as the base for the computations of probability amplitudes. The computer model supports two modes for the computation of the probability amplitudes: (1) computation according to standard QFT, and (2) computation according to a proposed functional interpretation of quantum theory.

Keywords—Computational Modeling, Simulation of Quantum Theory, Quantum Field Theory, Quantum Electrodynamics.

I. INTRODUCTION

The development of QTModel started with the objective to demonstrate the key concepts of quantum mechanics through simulation of the major (Gedanken-) experiments described in the literature on quantum theory (QT). Thereby, the details of the experiment setup should be configurable by the user. However, it was soon recognized that these objectives imply the modeling of interactions between particles. This resulted in the necessity to include QFT besides the basic quantum mechanics.

Support of the general QT concepts (and of the related Gedanken-experiments) also requires support of the major QT principles. With some of these experiments, however, problems showed up in mapping QT principles to a computer program. Computability has also been found to be a problem with some of the experiments. Typically, the list of possible processes contains processes which, when more details are specified, such as energies, cannot occur in reality. QTM will detect this, at the latest, when the probability (amplitude) is calculated. Certain cases of impossible processes will already be detected prior to the probability amplitude calculation.

II. STARTING QTMODEL

When the user starts QTModel she has to select one of the following options:

1) Define or run a general QT application
   This option is not described in this paper.
2) Define and run QED process
3) Define and run QED + Weak Interaction process

When "QED" or "QED + Weak Interaction" is selected, QTModel continues with the definition of the initial configuration.

III. DEFINITION OF THE INITIAL CONFIGURATION

The user interface window shown in Fig. 1 supports the definition of an initial configuration.

Besides serving as a useful teaching and studying aid, QTModel can also play a role in experimentation with new algorithms for the computation of QT/QFT predictions. QTModel started with emphasis on quantum electrodynamics (QED) and weak interactions. Extension to support strong interactions are in progress.

QTModel offers the following functions:

- Definition of an initial set of particles with their relevant attributes
- Determination and listing of the possible processes leading to alternative output configurations
- For a selected process, listing of the subprocesses, i.e. alternatives resulting in the same output configuration
- Generation of the Feynman diagram for a selected subprocess
- Generation of the term for the S-matrix element for a selected subprocess
- Evaluation of the probability amplitude and cross section for a selected process or subprocess

Details on these functions are described below.

IV. DETERMINATION AND LISTING OF THE POSSIBLE PROCESSES

After the initial configuration has been specified, the possible processes which start with the specified initial configuration can be listed by use of the "List" button. Each process is uniquely identified by its output configuration. The list of possible processes contains processes which, when more details are specified, such as energies, cannot occur in reality. QT will detect this, at the latest, when the probability (amplitude) is calculated. Certain cases of impossible processes will already be detected prior to the probability amplitude calculation.
V. LISTING OF THE SUBPROCESSES

Typically, for a given process, there exists multiple alternatives, called subprocesses, resulting in identical output configuration. The list of subprocesses for a selected process may be displayed by use of the "Subprocesses" button. In the example shown in Fig. 1, selection of the first process in the list ("$\rightarrow$ BhabhaScattering $\rightarrow$ Out: $e^-, e^+$"), with Iterations = 2 and P-order = 2, results in the list shown in Fig. 2.

VI. GENERATION OF THE FEYNMAN DIAGRAM

After the selection of a subprocess, the Feynman diagram for the subprocess can be displayed by pressing the "Draw" button. Fig. 3 shows two Feynman diagrams for Bhabha scattering.

If the appearance of the generated Feynman diagram is not completely satisfying for the user, certain drawing options and the placement of vertexes may be varied by use of the "Options" button. As shown in Fig. 4, the drawing options enable specification of:

- diagram flow either from "Bottom to top" or from "Left to right"
- whether names should be displayed for lines and vertexes
- whether names for the momenta should be displayed
- whether particle names should be derived from the particle type
- the title to be displayed with the diagram
- rearrangement of the diagram layout by changing coordinates of vertexes. The coordinates shown and the possibly modified coordinates refer to the "bottom to top" drawing.

VII. REDUCE SUBPROCESSES

The list of subprocesses generated by QTModel for a given process usually contains more subprocesses than the literature on QFT distinguishes for the respective process. The initial list generated by QTModel may be reduced by use of the "Reduce" button shown in Fig. 2. QTModel reduces the list of subprocess according to three criteria.

1) eliminate subprocesses with less vertexes than requested by P-order,
2) eliminate subprocesses where some of the input particles do not interact, and
3) eliminate subprocesses which are equivalent.

Diagrams are considered equivalent if they result in identical terms and probability amplitudes.
VIII. GENERATION OF THE S-MATRIX TERM

When generation of the S-matrix term is requested, a window is displayed which allows the specification of the names used in the generated S-matrix term. QTModel initializes the input fields by default names. Depending on the button pressed, the term is generated and displayed either in TeX format or in HTML format. In TeX format the term generated for Diagram A shown in Fig. 3 looks as follows:

\[ M = (-ie)^2 \bar{v}(\vec{p}_2, s_2) \gamma_\mu u(\vec{p}_1, s_1) (-ig_\mu\nu/(p_1 + p_2)^2) \bar{u}(\vec{p}'_1, s'_1) \gamma_\nu v(\vec{p}'_2, s'_2) \]

This cryptic notation is not directly readable by the user. In order to make it readable the user has to include it in a TeX processor. The above text would then result in the following:

\[ M = (-ie)^2 \bar{v}(\vec{p}_2, s_2) \gamma_\mu u(\vec{p}_1, s_1) (-ig_\mu\nu/(p_1 + p_2)^2) \bar{u}(\vec{p}'_1, s'_1) \gamma_\nu v(\vec{p}'_2, s'_2) \]

Similarly, generated HTML text has to be included in a HTML processor (e.g. Internet browser) to make it readable.

IX. EVALUATION OF THE PROBABILITY AMPLITUDE

The probability amplitude may be evaluated for a given process or for a selected (set of) subprocesses. If it is invoked without selecting a set of subprocesses, QTModel determines the set of applicable subprocesses according to the QFT rules.

When the probability amplitude for a complete process (e.g. Bhabha scattering) is to be evaluated, this is accomplished by the superposition of the applicable subprocesses. This may mean summation or subtraction of the probability amplitudes.

As the major result of the "Evaluate" function, the probability amplitude for a (set of) subprocess(es) or a complete process is evaluated. Further results, such as the scattering probability, the differential or total cross section or the decay rate may be derived from the probability amplitude and are provided by QTModel.

Before the probability amplitude can be evaluated by QTModel, further parameters have to be provided by the user. Some global parameters (e.g. total energy) may be entered at the window shown in Fig. 5. Attributes such as momentum, helicity and position of the individual external particles are entered by pressing the "Particle Details" button. Particle details may be omitted if global parameters such as energy and angle are specified, and the momentum of the in-particles is in z-direction and a two body rotation symmetrical process can be assumed. The determination of the attributes of the individual particles then depends on whether or not "CoM frame" (center of mass frame) is requested. If "CoM frame" is not requested, "Lab frame" is assumed. Specification of parameter ranges for the energy or the scattering angle results in curves displayed graphically (see for example Fig. 6).

The window also supports specification (i.e. changing) the title for the (sub-)process being evaluated. This may be useful if the evaluation results in curves being displayed and then copied to text documents.

The evaluation of the probability amplitude can be requested either by computations based on standard QFT (Button "Std-QFT") or by execution according to the functional interpretation (Button "Funct.Interp.").

1) Computation in Momentum Space: Computation in momentum space is the typical kind of computation described in QFT textbooks (see [2], [3], [4], [5]). Special case specifications such as "center of mass frame", "momentum in z-direction" and "rotation symmetric" are used just for easier determination of the initial parameters (e.g. momentum). They have no effect on the subsequent evaluation of the probability amplitude. If the spin of the particles is not explicitly specified, it is assumed to be "undefined" and this means that the average
or the sum of the possible spin combinations is evaluated.

If ranges are specified for the total energy, or for the scattering angle, the evaluation results in curves displayed by QTModel. For example, the result of the evaluation of Bhabha scattering with parameters shown in Fig. 5, is shown in Fig. 6. As can be seen in Fig. 6, three types of evaluation results may be requested by pressing the respective button. If "Probability" is requested, the main result of the evaluation, the square of the probability amplitude \( |M|^2 \), is shown. "Diff.CrossSection" shows the differential cross section. "TotalCrossSection" is the integration of the differential cross section for the specified range of scattering angles.

X. SIMULATION EXAMPLES

The following describes major simulation examples. The main criteria for the selection of the examples was the availability of comparable computation results in literature (the literature sources are not mentioned in detail).

A. Tauon pair creation, \( e^- e^+ \rightarrow \tau^- \tau^+ \)

The scattering of electron - positron normally results in an electron - positron pair with changed momentum (i.e. direction of movement). When the initial electron - positron pair has a high enough energy, the scattering may also result in different particle types, for example tauons. The example starts by specifying as the initial configuration an electron \( e_1 \) and a positron \( pos \) as shown in Fig. 1. The list of possible processes obtained by pressing the "List" button contains as the last entry "Out:tau-,tau+" as shown in Fig. 7 (in Fig. 1 the list would have to be scrolled down). Selection of the "Out:tau-,tau+" process and pressing "Subprocesses" leads to a window like the one shown in Fig. 2. However, with the tauon pair creation, the list of subprocesses contains just one entry, namely "In:e-, e+ Out: tau-, tau+, subprocess: S5 ... \( \rightarrow (\tau u^- , \tau + u) \) ".

For this subprocess QTModel supports the generation of the scattering matrix term, the display of the Feynman diagram, and the evaluation of the scattering probabilities and cross section. Pressing the "Draw" button in Fig. 2 results in the Feynman diagram shown in Fig. 8.

The diagram shown in Fig. 8 is similar to Diagram A for Bhabha scattering (see Fig. 3). The term generated when pressing "GenTerm" appears as

\[
M = (-ie)^2[\bar{v}(p_2, s_2)\gamma_\mu u(p_1, s_1)](-ig^{\mu\nu}/(p_1 + p_2)^2)[
\bar{u}(p(\tau u^- , 0), s_3)\gamma_\nu v(p(\tau u^+, 0), s_4)].
\]

Invocation of the "Eval.Ampl." function (via the respective button) leads to the window shown in Fig. 5 with parameters according to the present example. As an example, let us assume we are interested in the differential cross section for the total energy 10 GeV and the range of scattering angles between 0 and 180 degrees. These parameters can be directly entered; there is no need to specify the details for the ingoing and outgoing particles. Pressing "Std-QFT" invokes the evaluation of the probability amplitudes and the differential cross section. The result of the evaluation is shown in Fig. 9.

B. Tauon pair creation, \( e^- e^+ \rightarrow \tau^- \tau^+ \), including weak interaction

The tauon pair creation described above disregards weak interaction. When weak interactions are included (by starting QTModel accordingly), there is a further process which has to be considered. For the process shown in Fig. 10 the virtual
Bhabha scattering is selected by specifying an initial configuration consisting of an electron and a positron. QTModel generates the list of possible processes as shown in Fig. 1. In the resulting list of possible processes, the first is the one where the output configuration is identical with the input configuration.

Selecting the first process in the list ("- > BhabhaScattering- > Out : e- : e+") and pressing the "Subprocesses" button leads to the window shown in Fig. 2. The list of subprocesses shown in this figure shows six subprocesses. With the listed subprocesses 1., 2., and 5. the involved particles (electron and positron) do not interact, which makes them irrelevant for further QFT modeling. The list also contains subprocesses 3. and 4. which, for the purpose set of QFT computations are considered equivalent. This classification of the subprocesses may be obtained by use of the "Reduce" button.

Further functions provided in the window shown in Fig. 2 are "Draw", "Gen.Term" and "Eval.Ampl.". Draw and Gen.Term must be applied to a specific subprocess. Selection of individual subprocesses or subprocesses selected by the user, or to the whole process (Bhabha scattering) . Selection of individual subprocesses or sets of subprocesses may be of theoretical interest, but makes sense only if the user knows how to interpret the results of the evaluation. Normally, "Eval.Ampl." should be applied to the whole process.

Eval.Ampl for the whole Bhabha scattering process leads to the window shown in Fig. 5. Before presenting this window, QTModel has to determine which of the subprocesses listed in section 10.1 to obtain the total amplitude. This amplitude has to be added to the amplitude described above in section 10.1 to obtain the total amplitude.

\[ M_{\text{total}} = M_{\text{QED}} + M_{\text{weak}}. \]

The "Eval.Ampl." function now considers both diagrams. Choosing as evaluation parameters an energy range of 5 to 100 GeV and an angle of 90 degrees results in the differential cross section curve shown in Fig. 11. The peak at the low energy is due to the QED contribution. The weak interaction through Z0 becomes significant at the high energies.

**C. Bhabha Scattering**

This section summarizes the various pieces related to Bhabha scattering which has been the guiding example throughout this paper. Bhabha scattering means electron-positron scattering with both the electron and the positron surviving with possibly changed momentum direction.

The "Eval.Ampl." function now considers both diagrams. Choosing as evaluation parameters an energy range of 5 to 100 GeV and an angle of 90 degrees results in the differential cross section curve shown in Fig. 11. The peak at the low energy is due to the QED contribution. The weak interaction through Z0 becomes significant at the high energies.

\[ M = (-ie)^2 \left[ v(p_2, s_2) \gamma^\mu u(p_1, s_1) \left( -ig_{\mu\nu}(p_1 + p_2)^2 \right) \right], \]

The most elaborate function of QTModel is "Eval.Ampl.". The function may be applied to individual subprocesses, to sets of subprocesses selected by the user, or to the whole process (Bhabha scattering). Selection of individual subprocesses or sets of subprocesses may be of theoretical interest, but makes sense only if the user knows how to interpret the results of the evaluation. Normally, "Eval.Ampl." should be applied to the whole process.

Eval.Ampl for the whole Bhabha scattering process leads to the window shown in Fig. 5.
The formula is to the formula mentioned in QFT literature, for example [3]. The energy relationship of the outgoing photon to the ingoing photon is determined according to individual particle attributes. The energy relationship of the two subprocesses where diagrams are shown in Fig. 3 have to be included, and that the respective probability amplitudes have to be subtracted:

\[ M_{\text{total}} = M_A - M_B \]

For the more detailed parameters in the example it is assumed that initial momenta are in z-direction, the center-of-mass frame, and rotation symmetry. When this is marked with the window shown in Fig. 5, it is sufficient to specify only the total energy (5 GeV) and the scattering angle (45 - 130 degree). By use of the "Std-QFT" button, the following can be displayed: the distribution of probabilities, the differential cross sections, and the total cross section. Fig. 6 shows the distribution of the differential cross section.

### D. Compton Scattering

Compton scattering means photon - electron scattering, \( e^- \gamma \rightarrow e^- \gamma \). Specification of the initial and final configuration is trivial, and therefore not further described here. For the evaluation of probability amplitudes and cross sections, the two diagrams shown in Fig. 12 are applicable. This time, however, the respective probability amplitudes have to be added.

\[ M_{\text{total}} = M_A + M_B \]

with

\[ M_A = (-ie)^2 \epsilon_{\nu}(p_2, \lambda)\epsilon_{\mu}(p_2', \lambda)[\bar{u}(p_1', s_i)]\gamma^\nu i/(\gamma_i(p_1 - p_2') - \mu)\gamma^\mu u(p_1, s_i) \]

\[ M_B = (-ie)^2 \epsilon_{\nu}(p_2, \lambda)\epsilon_{\mu}(p_2', \lambda)[\bar{u}(p_1', s_i)]\gamma^\nu i/(\gamma_i(p_1 + p_2) - \mu)\gamma^\mu u(p_1, s_i) \]

For photon-electron scattering, the center-of-mass-frame does not make sense. Therefore, "CoM frame" is turned off at the respective checkbox shown in Fig. 5. If global parameters are specified as energy = 0.511 MeV and the range of angles = 0 to 180 degrees, QTModel computes the values for the individual attributes. The energy relationship of the outgoing photon to the ingoing photon is determined according to the formula mentioned in QFT literature, for example [3]. The formula is

\[ \bar{\omega}' = \frac{\bar{\omega}}{\gamma > \cos \theta} \]

where \( \theta \) is the scattering angle.

### E. Moeller Scattering

Moeller scattering means scattering of two electrons, \( e^- e^- \rightarrow e^- e^- \). Specification of the initial and final configuration is similar to that described above for Bhabha scattering. For the evaluation of probability amplitudes and cross sections, the two diagrams shown in Fig. 14 are applicable. The diagrams may be obtained by use of "Draw" in Fig. 2.

Evaluation of the probability amplitudes for the energy = 0.511 MeV and the range of angles 0 to 180 degrees results in Fig. 13. The result is in accordance with the results obtained from the Klein-Nishina formula (see [3]).

![Diagram of Compton Scattering](image1)

![Diagram of Moeller Scattering](image2)
The results of evaluation of probability amplitudes for energy = 500 MeV and the range of angles 5 to 175 degrees are shown in Fig. 15.

F. Z0 Decay, Z0 → e−, e+

The Z0 particle belongs to the weak interacting particles. Z0 decays into fermion pairs (Z0 → e−, e+, or Z0 → τ−, τ+, or Z0 → μ−, μ+), neutrino pairs, or quark pairs. Here, decay Z0 → e−, e+ is described.

As the initial configuration, only a single particle, the Z0, has to be specified. When listing the possible processes (via List button, see Fig. 1), QTModel lists the possible Z0 decay processes. Besides the straightforward processes Z0 → e−, e+, Z0 → τ−, τ+, and Z0 → μ−, μ+, the list also contains processes containing more than 1 vertex, if P-order > 1. Selecting the entry “Z0Decay Out: e−, e+” and pressing “Subprocesses” leads to the possible subprocesses for the example chosen. With the present example the list contains just a single subprocess. Invocation of “Draw” shows the diagram shown in Fig. 16. Invocation of “GenTerm” provides the term for the evaluation of the amplitude as

\[ M = \epsilon_\mu (p z, \lambda) \bar{u}(p(\text{Electron0})) \frac{i g_\lambda \gamma^\mu (\epsilon_\nu - \epsilon_A \gamma^5)}{v(p(\text{Positron0}))} \]

"EvalAmpl" leads to the window shown in Fig. 17. As with the previous examples, there is no need to specify "Particle Details". Global specification of total energy and angle is sufficient for QTModel to evaluate the probability |M|^2. For example, specifying energy = 0 MeV and an angle = 0 delivers the decay rate = 0.07856 as shown at the bottom of Fig. 17.  

XI. NOVEL ALGORITHMS

A. Computations according to Standard QFT

The majority of functions of QTModel described in the preceding sections are transformations of the equations given in textbooks on QFT such as [2], [3], [4],and [5]. Although the algorithms employed in QTModel cannot be considered as novel in this sense, the program uses a general (numerical) computation approach rather than a collection of the specific case formulas (such as, for example, the Klein-Nishina formula for Compton scattering) available in QFT.

B. Computation in Coordinate Space

With QFT, this means that the initial and final configuration are specified in terms of particle positions. QTModel applies computation in coordinate space if the user provides the position specifications under "Particle Details" in Fig. 5. In addition, in this case the program requires that the distribution of momentum \( \psi(p) \) and of the position \( \psi(x) \) are specified as Gauss-distributions. The window supporting "Particle Details" (not shown in this paper) allows the specification of a Gauss-distribution for the momentum. The position distribution can be specified separately for the initial and final configurations.

1The energy specification is ignored for decay processes. Different values for energy and angle would deliver the same decay rate, because the decay rate is independent of energy and angle.
The complete wave function $\psi(x,y)$ is then obtained by

$$\psi(x,y) = \int dx \ G(x,y) \ \psi(x)$$

where $x$ is the end coordinate and $y$ is the start coordinate. Using the momentum distribution $\psi(p)$ instead of the position distribution $\psi(y) = \frac{1}{\sqrt{2\pi}} \int d^4p' \ e^{ip(y-x)} \psi(p')$ leads to

$$\psi(x) = \int dy \ \frac{1}{\sqrt{2\pi}} \int d^4p \ e^{ip(y-x)} \psi(p') \ e^{ipx} \delta(p-p')$$

Applying the $\delta$ -function substitution rule

$$\int dy \ e^{ip(y-x)} = \delta(p-p')$$

this may be transformed to

$$\psi(x) = \int d^4p \ e^{-ipx} \frac{1}{\sqrt{2\pi}} \int d^4p' \ e^{ip(y-x)} \psi(p')$$

or more generally again

$$\psi(x) = \int d^4p \ e^{-ipx} (\frac{1}{\sqrt{2\pi}} \int d^4p' \ e^{ip(y-x)} \psi(p'))$$

This equation (1) is used by QTModel for the computation in coordinate space for the propagation of a single particle. Differing from the "pure" coordinate space computation, where the integral on $p$ has to vary from $-\infty < p < +\infty$, with QTModel and its request for a non-sharp Gauss-distribution for the position, the integral has to cover only a limited range given by the distribution $\psi(p) \neq 0$.

Similar but more sophisticated considerations apply to computation for scattering in coordinate space.

C. Evaluation Based on Functional Interpretation of QT

As mentioned in the Introduction, QTModel's support of the major QT concepts and Gedanken-experiments touches on fundamental principles of QT. However, since some of these principles are formulated in natural language, which cannot easily be mapped to precise mathematics or a computer program, the author has looked for interpretations of these principles that are consistent with computability. For the result of this work see "A Functional Interpretation of Quantum Theory" described in [6]. As the title suggests, the emphasis in this functional interpretation will be on describing what actually happens. Key features dealt with are:

- coarse graining for attributes and path subdivision,
- particle/wave fluctuations taking the role of virtual particles,
- transition from probabilities to facts not tied to measurements, and
- path collections in support of entanglement.

To invoke this functional interpretation, press "Funct.Interpr." (see Fig. 5). As far as the QFT simulation dealt with in the present paper is concerned, the most significant difference between the "Std. QFT" and the "Funct.Interpr." is that the latter is not based on Feynman diagrams and fermion chains. For further details on this functional interpretation see [6]. The main purpose of including "Funct.Interpr." at this stage is to verify it’s results against those obtained with "Std-QFT" evaluation. In the next phase of this project, functional interpretation will be a prerequisite for general support of QT concepts.

XII. Conclusions

QTModel is capable of running major QFT processes such as Bhabha, Moeller, Compton scattering, plus tauon pair creation (with or without weak interaction) and Z0 decay. The results generated are in agreement with the computation results published in the literature on QFT. QTModel’s general approach for the specification and evaluation of the QFT processes supports the simulation of a large variety of further QFT processes not shown in this paper.

The implementation of QTModel is not yet complete in all the areas targeted with the initial objectives. A major area that is still missing is extended support of computations in coordinate space. Support of computations in coordinate space and extended support of the functional interpretation are major prerequisites for support of the major QT concepts and Gedanken-experiments as planned with the original objectives.

Another planned extension is support of higher orders of perturbation. It is expected that the numerical computation techniques already applied with QTModel may offer alternative solutions to standard QFT renormalization and regularization techniques.

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Hans H. Diel was for many years a leading software architect in an IBM research and development laboratory, and has worked as a freelance software development consultant. The work described in this paper is the result of his interest in the simulation of quantum theory. (See http://www.hans-diel.de.)