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Problems and Possible Solutions with the Development of a Computer Model of Quantum Theory

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Abstract—A computer model of Quantum Theory (QT) has been developed by the author. Major goal of the computer model was support and demonstration of an as large as possible scope of QT. This includes simulations for the major QT (Gedanken-) experiments such as, for example, the famous double-slit experiment.

Besides the anticipated difficulties with (1) transforming exacting mathematics into a computer program, two further types of problems showed up, namely (2) areas where QT provides a complete mathematical formalism, but when it comes to concrete applications the equations are not solvable at all, or only with extremely high effort; (3) QT rules which are formulated in natural language and which do not seem to be translatable to precise mathematical expressions, nor to a computer program.

The paper lists problems in all three categories and describes also the possible solutions or circumventions developed for the computer model.

Keywords—Computability, Foundation of Quantum Mechanics, Measurement Process, Modeling.

I. INTRODUCTION

THE aim of the computer model QTModel is the provision of a reasonably general computer model of quantum theory. There exist numerous computer programs which calculate the expected results for special experiments. Compared to these programs QTModel aims at more generality. In literature on QT, the key concepts of QT are often explained (and sometimes even substantiated) by Gedanken-experiments. As a proof for the desired generality, QTModel should be capable of simulating most of the Gedanken-experiments described in literature. Thereby, the details of an experiment set-up should be configurable by the user of QTModel.

The goal of supporting generality, together with the goal of supporting detailed user-defined configuration of experiments resulted in the need to include in QTModel the modeling of interactions between particles. This results in the need for supporting quantum field theory (QFT) besides the overall quantum mechanics. Support of quantum field theory adds further mathematical challenges to the computer model. QFT is defined in terms of exacting precise mathematics. However, the respective equations can often be solved only for special cases and/or with extremely high effort.

When the project started it was clear to the author that this will not be a trivial task. Besides the anticipated difficulties in transforming the exacting mathematics of QT/QFT into a computer program, further problems showed up which could not be foreseen by studying textbooks on QT and QFT. There are several QT rules which are formulated in plain natural language and which do not seem to be translatable into mathematical equations. Such rules are also difficult or impossible to translate to a computer program.

As is widely known, QT contains some strange concepts. One might expect that concepts such as entanglement are further examples which can hardly be supported by a computer model. This turned out not to be the case. [1] In section V. it is described why some major "strange" QT concepts do *not* represent a problem for the QTModel implementation.

Below, the major problem types which faced QTModel are described, namely (1) "normal" problems, (2) QFT areas with poor computation ability, (3) QT rules which cannot be translated to mathematics, and (4) "no problems". The description also contains the solutions chosen for QTModel. The major solution categories are

- the feature which causes the problem is not supported by QTModel
- the feature which causes the problem is supported by QTModel only to a limited degree. Work continues to extend support of the feature.
- a "functional interpretation" of QT/QFT has been developed which enables support of the feature by a computer model.

The QTModel solutions are described only very roughly. More details can be found in [2] and [3].

II. THE "NORMAL" PROBLEMS

"Normal" problems, i.e. problems which one has to expect with the development of a computer program for an area of science, are obviously not the major subject of this paper. Therefore, only some major problem areas are mentioned here:

- The quality of text books on QFT, when different text books seemed to be conflicting.
- Difficulties in finding comparable data which allows a verification of the results generated by QTModel.
- Finding out which Gedanken-experiments have been verified by real experiments.

III. QFT AREAS WITH POOR COMPUTABILITY

For reasons described above, quantum field theory is the central part of the modeling of general QT. QFT is based on an impressive mathematical framework. It was a surprise to the author that the availability of this mathematical base does not

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[1] This does not mean that the computer simulation makes the concepts less strange.

automatically imply computability in all areas of the theory. There are mainly three areas of QFT where computability is a problem:

A. Computation in Coordinate Space

Computations of probabilities, or cross sections for the results of QFT processes such as scatterings or decays, may be performed in momentum space or in coordinate space. Computation in momentum space requires that the momenta for the initial and final states of the particles are specified. Likewise, computation in coordinate space requires that the positions of the particles are specified. Studying textbooks on QFT (see for example [9], [6],[7], [5]) , at first glance it looks as if computations in momentum space and computation in coordinate space are two alternatives on equal footing. The fact that computation in coordinate space is poorly described in these textbooks may be due to the larger applicability of computations in momentum space. After deeper study, it becomes clear that computations in coordinate space can be very difficult and may lead to equations for which solutions do not exist at all, or can only be found with special cases.

When it may be said that computations in coordinate space are poorly described and understood, this is even more true for the general case, computations where momenta as well as positions are given with specific distributions. QT requires that the momentum and the position assigned to particle have a certain distribution, for example a specific Gauss-distribution. Calling the distribution of the momentum $\psi(p)$ and that of the position $\psi(x)$, a distribution width $\Delta_d(p)$ and $\Delta_d(x)$ can be defined. QT states that $\psi(p)$ and $\psi(x)$ are correlated such that one can be determined from the other via Fourier-transformation

(1) $\psi(p) = Fourier(\psi(x))$ and vice versa.

Furthermore, holds

(2) $\Delta_d(p) \cdot \Delta_d(x) \geq \hbar/2$. [2] [3]

QFT computation in momentum space means that the momenta have exact values ($\Delta_d(p) = 0$), which means the possible position values are completely arbitrary ($-\infty < x < +\infty$). For computations in coordinate space the positions are exactly known, and the momenta are completely undefined. Directions for computation for the general case with $\Delta_d(p) \geq 0, \Delta_d(x) \geq 0$ could not be found in the literature.

Besides the mathematical difficulties associated with the treatment of computations in coordinate space and of the general case, the main reason for the lack of computation directions is probably the fact that, computations in momentum space are sufficient for most of the typical work of QFT physicists. For the provision of a computer model of QT/QFT which has, like QTModel, the objective to support the largest possible scope of QT/QFT exclusion of computations in coordinate space and the general case would also exclude simulation of many Gedanken-experiments (such as the double-slit experiment).

1) QTModel Solution:: With the search for a solution that supports computation in coordinate space in QTModel, it was, first of all, decided to aim at supporting the general case. Support of computation in coordinate space is then just the extreme special case of the general solution. The users of QTModel can invoke coordinate space computation only, if they specify a non-sharp distribution of the momentum. The (non-flat) position distribution can then be determined by QTModel via Fourier-transformation.

Support of the general case does not seem to be more difficult than support of "pure" coordinate space computation. It does not seem to be much easier, either. The remaining difficulties in handling nested integrals over infinite complex spaces will be tackled with numerical computation approaches and variants of Monte Carlo simulation methods.

B. Computation of Higher Orders of Perturbation

The main approach for the computation of the probabilities for the results of QFT processes (e.g. scatterings, decays) is the so-called perturbation approach invented by Feynman and Dyson. The perturbation orders, resulting in improved precisions of the computation results, are characterized by an increased number of intermediate points (= vertexes) on the paths from the initial state towards the final state. The computation for the lowest order of perturbation is straight forward. Higher orders of perturbation can be very difficult. In terms of the related Feynman diagrams, the higher orders of perturbation often result in loops. In terms of mathematical equations, the loops mean integrals in infinite complex space. Often these integrals are diverging, leading to results which are physically senseless. With standard QFT the diverging integrals are tackled by very sophisticated techniques called regularization and renormalization. These techniques are not suited for implementation by a computer program, which aims at supporting the general cases.

For the achievement of an acceptable precision for the QFT computation, the higher orders of perturbation are required primarily with scatterings involving strong force (i.e. QCD).

1) QTModel Solution:: QTModel uses numerical methods for the computation of integrals. The methods implemented recognize when the integrals are diverging and will then stop further integration. This may result in certain experiments and certain areas of QT not being supported. The major area which is therefore excluded from support by QTModel is QCD.

C. Computations for Bound Systems

Predictions for the behavior of bound systems, such as an atom, a nucleus, or a hadron, can be computed with QFT for special situations only, and only with considerable high effort. QFT includes some theory and considerations on bound systems (see [9], [8], [5]), but this does not include a complete and consistent description of the total system in terms of QFT constructs such as Feynman diagrams, etc.. In [9] S.Weinberg writes "It must be said that the theory of relativistic effects and radiative corrections in bound states is not yet in entirely satisfactory shape".

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[2] This may be considered as a special variant of Heisenbergs uncertainty relation $\Delta p \cdot \Delta x \geq \hbar/2$.

[3] assuming the appropriate definition of Δ_d.

1) QTModel Solution:: The construction and running of bound systems is not supported by QTModel. As a future extension, it is envisaged to do experimentation with QTModel to achieve a better understanding of the formation of bound systems based on QFT processes.

IV. QT RULES WHICH CANNOT BE TRANSLATED INTO MATHEMATICS

Although QT is founded on an extensive and exacting mathematical framework, and many important discoveries (e.g. of new particle types) were the result of mathematical reasoning, there are a few places which are formulated in plain natural language and which do not seem to be translatable into mathematics. For the computer model the real problem, of course, arises when a QT rule which needs to be reflected in the computer model cannot be translated into a computer program. However, it seems that rules which cannot be translated into mathematics also cannot be translated into a computer program. [4]

A. Which Path Did the Particle Take ?

With the early Copenhagen interpretation of QT, there was a refusal to talk about what happens before a measurement takes place. This kind of positivistic view was mainly justified by the fact that classical notions of physics are no longer applicable here. A famous example is the question of which slit does the electron go through with the double-slit experiment. Indeed, it may not be reasonable to ask about *the* path taken by a particle before a measurement occurs, but this should not justify disallowing any questions about the dynamic evolution of the particle (or its wave function) prior to a measurement.

1) QTModel Solution:: QTModel interprets QT in such a way that the particle, represented by its associated wave always goes through both slits. However, depending on the availability of measurement interactions on a path, only one of the paths may survive after the measurement interaction. [5]

B. When Are Probabilities As Opposed To Probability Amplitudes To Be Added ?

One of the basic features of QT is that the probability of an event for which multiple alternative paths are possible is a function of the superposition of the wave functions of the multiple paths. Superposition means summation of the probability amplitudes of the wave functions. In cases where there is no superposition, the probabilities for the multiple paths have to be added, which means the classical (i.e. non-QT) behavior.

The rule for deciding when probabilities as opposed to probability-amplitudes are to be added is one of the basic laws of QT. In [4], page 1-13 Feynman phrases it as follows:

"When an event can occur in several alternative ways, the probability amplitude for the event is the sum of the probability amplitudes for each way considered separately. There is interference:

$\Phi = \Phi_1 + \Phi_2$

$P = |\Phi_1 + \Phi_2|^2$

If an experiment is performed which is capable of determining whether one or another alternative is taken, the probability of the event is the sum of the probabilities for each alternative. The interference is lost.

$P = P_1 + P_2$ "

(end of citation)

This rule, or some alternative one, has to be implemented by any computer model which aims at supporting a reasonable set of the classical QT Gedanken-experiments, such as the double slit experiment. With the authors attempt to incorporate this rule into QTModel [6] , it was found that this was not possible. The rule is either not precise enough, or circular. An alternative, somewhat more concrete phrasing of the above rule would be: The probability amplitudes have to be added (i.e. are in superposition) unless the wave function collapses; and a wave function collapses if *through a kind of measurement* it is possible to determine that a particular path is taken. However, when exactly a situation may be considered as representing a measurement is one of the open questions of the unresolved measurement problem (see below).

1) QTModel Solution:: It was concluded that, in order to obtain a rule which is translatable to mathematics (and thereby also to a computer program), it is necessary to obtain a model on the interaction *process* leading to the abortion of the superposition. A "functional interpretation of QT/QFT" has been developed with this goal. It is described in more detail in [2].

C. The Measurement Problem - What Happens When *a Measurement Takes Place ?*

The so-called "measurement problem" was identified as one of the major open issues of QT soon after the formulation of quantum mechanics. There is no agreed-upon theory on what causes a measurement, and what exactly happens when a measurement takes place. Various so-called interpretations of QT (e.g. the "many worlds" interpretation) are related to this problem.

At first glance it is not clear why the unsolved measurement problem should impede a computer model of QT/QFT. However, given the ambitious goals of QTModel (of supporting a large set of QT applications and experiments) two reasons for the need for some solution to the measurement problem can be seen:

- QTModel would be more complete if it's modeling of QT/QFT did not end at the point of measurement, but if the measurement process itself were included. On the other hand, one may argue that, if QT does not yet have a clear picture on the measurement process, why should QTModel provide this ?
- Besides measurements representing the end of a QT/QFT experiment, there are, according to the QT interpretation

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[4] The mathematical theory on computability says that the opposite is not true.

[5] This interpretation does not seem to be in conflict with current discussions of the double-slit experiment in literature. However, it is usually not explicitly described this way either.

[6] The problem has already been detected with an earlier project, see [1].

favored by the author, many measurement-like types of interactions which have to be supported by QTModel. An example of such a measurement-like interaction is the interaction which leads to the abortion of the superposition (see above). Without a functional interpretation of measurement-like interactions, it will not be possible to support a large set of the classical QT Gedanken-experiments.

1) QTModel Solution:: As a generalization of what is described above in section IV.B. "When are probabilities as opposed to probability amplitudes to be added ?" the proposed functional interpretation of QT/QFT includes a model of QT measurements. Details on the functional interpretation are described in [2].

V. NON-PROBLEMS

There are several concepts in QT which are commonly viewed as being strange or even mysterious. One would expect that such features represent a problem for a computer model. Nevertheless, the items listed below are classified as "Non-Problems" for different reasons. Two of them (the uncertainty principle and the principle of complementarity) are not a problem for QTModel because QTModel does not support the simulation of experiments where these features are explicitly accessed. The third one, entanglement, is not a problem, because, despite its strangeness, it is mathematically well-defined.

A. The Uncertainty Principle

Heisenberg's famous uncertainty principle occurs with many Gedanken-experiments for one of the following purposes:

- It is used to argue that, because of the uncertainty principle, some other principle (for example the ones addressed in section IV.) holds true (in the specific case).
- Gedanken-experiments are often used to support the uncertainty principle itself.

The direct reference to the uncertainty principle, in its general version, is not supported by QTModel. However, sometimes the uncertainty principle

(3) $\Delta p \cdot \Delta x \geq \hbar/2$

is explained by associating Δp and Δx with the width of the wave functions $\psi(p)$ and $\psi(x)$. As described in section III.A., (2) may indeed be considered as a "lean" version of the uncertainty relation, (3).

1) QTModel Solution:: As described above, the reference to the uncertainty principle is not supported by QTModel. The inclusion of the "lean" version of the principle $\Delta_d(p) \cdot \Delta_d(x) \geq \hbar/2$ is implied with the overall QT/QFT logic and as such is supported by QTModel.

B. Principle of Complementarity

The principle of complementarity has been an important part of the Copenhagen Interpretation of QT. In present day literature on QT, it is still frequently used to explain certain Gedanken experiments.

1) QTModel solution:: QTModel does not support this concept, because (1) it is not seen how this principle could be mapped to mathematics or to a computer program, and (2) it is felt that the (Gedanken-) experiments which today are explained with reference to the principle of complementarity should have an explanation based on other, better founded QT laws.

C. Entanglement

Among the many concepts of QT that are hard to understand, and hard to believe, the concept of entanglement is probably the strangest. There are at present still experiments in progress trying to verify that it is indeed possible that the measurement on particle-1 instantaneously affects the possible outcomes of measurements on particle-2 with an arbitrarily large distance between the two particles. One might expect that such strange behavior, which seems to violate the principles of locality and/or causality, can hardly be simulated by a computer program such as QTModel.

1) QTModel Solution:: The reason why the simulation of entanglement does not represent a problem for QTModel is, that the concept of entanglement, in contrast to most of the problem areas mentioned above, is derived from exact mathematical formulations which are also suitable for the implementation by a computer program. Another reason for the absence of implementation problems is the fact that the non-locality required for support of entanglement does not provide a problem to a computer simulation. [7]

Saying that support of entanglement does not provide a problem to QTModel does not mean that it is a trivial function. The data representing particles has to be structured in such a way that it is suitable for support of entanglement. This leads to the introduction of "particle-collections" combining multiple (correlated) particles as well as multiple "particle-paths". For the entanglement mechanism there exists a variety of possible solutions ranging from (1) an expensive mechanism supporting perfect correlations, to (2) less expensive mechanism which support correlations to a less perfect degree, which however still violates Bell's inequality as predicted by QT.

D. Non-Determinism

With QTModel the non-determinism of QT appears in two two alternative ways, depending on the kind of output requested by the user:

- Instead of a single result value (e.g. scattering angle), the user wants to know the probabilities for a range of resultant values. This is the typical QTModel usage.
- With certain output alternatives (e.g. scattering or decay), the user may request QTModel to make the decision based on calculated probabilities. In such cases, QTModel will invoke a random number generator to make the decision.

1) QTModel Solution:: Both cases described above do not represent a problem to the QTModel implementation.

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[7] This assumes that entangled particles are represented in the same single storage.

VI. CONCLUSIONS

The major problems (actual and potential) for the development of a computer model of QT/QFT that supports the key concepts of QT such that the major Gedanken-experiments could be simulated, have been described. The solutions chosen by QTModel have also been roughly described. A more detailed description of the solutions can be found in [3]. Solutions to the problems described in section IV. ”QT Rules which cannot be translated into mathematics” resulted in the development of a ”functional interpretation of QT/QFT” (see [2]). It may be argued that the problems described in section IV. represent a deficiency of QT. A discussion of such an argument however would exceed the scope of this paper.

APPENDIX A
OVERVIEW OF QTMODEL

At present QTModel offers the following functions:

- Definition of an initial set of particles with their relevant attributes (e.g. position, energy, spin)
- 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 equations for the S-matrix element for a selected subprocess
- Evaluation of the probability amplitude and cross section for a selected process or subprocess

Extensions towards the original goals described in this paper are in progress. A detailed description of QTModel can be found in [3].

APPENDIX B
OVERVIEW OF THE FUNCTIONAL INTERPRETATION OF QT/QFT

A functional interpretation describes how things function. This implies the chronological order in which things happen. The functional interpretation proposed in [2] is based on QFT with the perturbation (Feynman) approach. Feynman diagrams are considered as a first step towards a functional interpretation. Key features of the proposed functional interpretation are

- criteria for deciding when interactions imply a collapse of the wave function
- 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.

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