Particle-based simulation approach for single-particle interference experiments: Application to double-slit experiments

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Abstract. We review recent progress in the development of event-by-event simulation algorithms that do not rely on concepts of quantum theory or probability theory but are nevertheless capable of reproducing the averages computed from quantum theory. The simulation approach is illustrated by applications to single-photon double-slit experiments. We demonstrate that it is possible to give a particle-only description of single-photon interference experiments without first solving a wave equation.

INTRODUCTION

Computer simulation is widely regarded as complementary to theory and experiment [1]. The standard procedure to construct a simulation model is to start from one or more basic equations of physics and to apply existing or invent new algorithms to solve these equations. Experience has shown that computer simulation is a very powerful approach to study a wide variety of physical phenomena but there are a number of physics problems, very fundamental ones, for which this approach fails, simply because there are no basic equations to start from.

Indeed, as is well-known from the early days in the development of quantum theory, quantum theory has nothing to say about individual events [2–4]. Reconciling the mathematical formalism that does not describe individual events with the experimental fact that each observation yields a definite outcome is referred to as the quantum measurement paradox and is the most fundamental problem in the foundation of quantum theory [3].

If computer simulation is indeed a third methodology of doing science, it should be possible to simulate the experimental observations on an event-by-event basis. For instance, it should be possible to simulate that we can see, with our own eyes, how in a two-slit experiment with single electrons, an interference pattern appears after a considerable number of individual events have been recorded by the detector [5]. To simulate such a experiments, we have two options

1. First solve the Schrödinger equation (numerically or analytically if possible). Then

use pseudo-random numbers to generate events according to the probability distribution obtained from this solution of the Schrödinger equation.

2. Do not make any reference to quantum theory but instead invent an Einstein local, causal process that generates events such that the frequency distribution of many events agrees with the one found in experiment (and with the solution of the Schrödinger equation).

In this paper, we do not consider the first option which, from a conceptual point of view is trivial. Indeed, as it first requires the solution of the Schrödinger equation (the Bohm trajectory description also requires knowledge of this solution), hence makes use of quantum theory, it has nothing meaningful to say about the mechanism that generates the events [3].

Therefore, we focus on the second option, namely the challenge to find algorithms that simulate, event-by-event, the experimental observations that, for instance, interference patterns appear only after a considerable number of individual events have been recorded by the detector [5], without making any reference to concepts of quantum theory. To head off possible misunderstandings, our work is not concerned with an interpretation or an extension of quantum theory nor does it affect the validity and applicability of quantum theory as such.

Logically speaking, there are three options to explain the observation of an interference pattern built up by successive, individual detection events:

1. One assumes that quantum theory provides the appropriate set of rules that correctly predicts the probability distribution to observe individual events but one refrains from trying to explain the observation of these individual events themselves. This "shut up and calculate expectation values" approach is, by construction, free of logical inconsistencies. It has proven to describe many different phenomena very well but does not offer an explanation for, not even any insight about, the process that actually produces the observed events.

2. One postulates that it is fundamentally impossible to give an explanation that goes beyond the description in terms of probability distributions to observe events. This is the prevailing position of contemporary quantum physics excluding, by postulate, the possibility that there may be explanations for the interference patterns observed in single-particle experiments in terms of individual events that do not make recourse to the probability distribution to observe these events.

3. One searches for a logically consistent explanation of the experimental facts, the observed detection events, that does not rely on the knowledge of the probability distribution to observe these events.

In this paper, we explore the last option and demonstrate that it is a viable one. Evidently, persuing this option requires modeling on a level that is not accessible to quantum theory. Our demonstration proves that the second option is untenable.

If we identify the registration of a detector click, the "event", with the arrival of a particle and assume that the time between successive clicks is sufficiently long such that these particles do not interact, we have to explain how the detection of individual objects that do not interact with each other can give rise to the interference patterns that are being observed. According to Feynman, the observation that the interference patterns are built
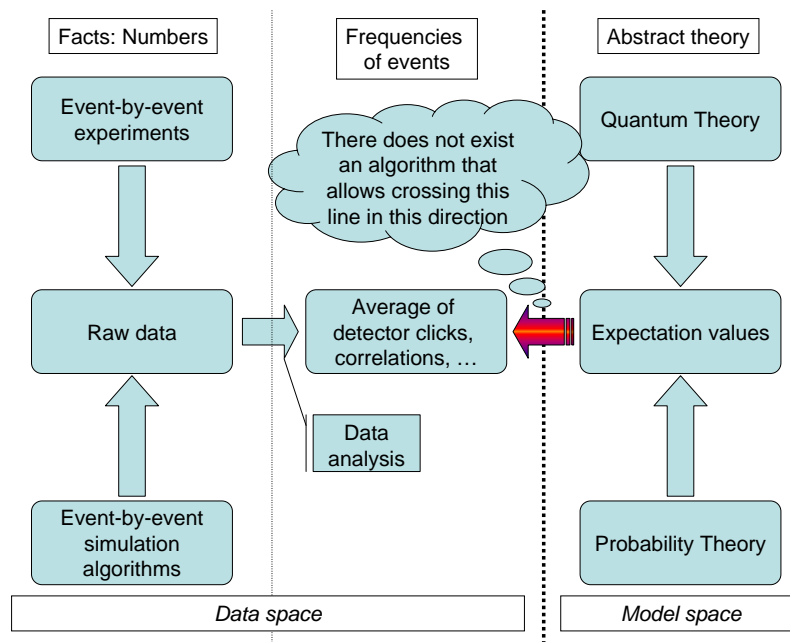
FIGURE 1. Logical relationship between data and theory.

up event-by-event is "impossible, absolutely impossible to explain in any classical way and has in it the heart of quantum mechanics" [6]. This paper indicates that this point of view needs to be revised.

It is not uncommon to find in the recent literature, statements that it is impossible to simulate quantum phenomena by classical processes. Such statements are thought to be a direct consequence of Bell's theorem [7] but are in conflict with other work that has pointed out the irrelevance of Bell's theorem [8–32]. A survey of the literature suggests that, roughly speaking, physicists can be classified as those who believe in the reasonableness of Bell's arguments, those who advance logical and mathematical arguments to show that a violation of Bell's (and related) inequalities does not support the far-reaching conclusions of the former group of physicists and those who do not care about Bell's theorem at all. The authors of this article belong to the second group. From the viewpoint of simulating quantum phenomena on a digital computer, Bell's no-go theorem is of no relevance whatsoever.

COMPUTER SIMULATION VERSUS EXPERIMENT AND THEORY

It is important to recognize that there are fundamental, conceptual differences between the set of experimental facts, their interpretation in terms of a mathematical model, and a computer simulation of the facts.

A graphical representation of the point of view taken in this paper is given in Fig. 1. On

the left, we have processes (experiments or computer simulations) that generate events. Each event is represented by one or more numbers, which we call raw data. Experience or a new idea provide inspiration to choose one or more methods to analyze the data. Typically, this analysis compresses the raw data into a few numbers (called averages and correlations in Fig. 1).

A theory such as Newtonian mechanics assigns real numbers to experimentally observable quantities. The relation between theory and experimental data is one-to-one and the theory is deductive in nature. Moreover, this theory contains all the necessary ingredients to construct a process that produces events (e.g. at time t the particle is at position x and has velocity v) that we observe in experiment. Thus, we place this theory on the data-space side in Fig. 1. The same can be said of Maxwell's theory, unless one tries to include the concept of a single photon.

Quantum theory assigns a probability, a real number between zero and one, for an event (= experimental fact) to occur [4, 7, 14]. By assigning probabilities to events, the character of the theoretical description changes on a fundamental level: Instead of deduction, we have to use inductive inference to relate a theoretical description to the facts [4, 33]. Therefore, quantum theory and probability theory belong to the model-space side in Fig. 1. From a computational perspective, a probabilistic theory does not contain the prescription of an algorithm that produces the events. In fact, this is a tautology: Any algorithm that executes on a digital computer is deterministic in nature, hence cannot model the random variables that appear in the probabilistic theory.

Crossing the line that separates the model space from the data space requires making the fundamental hypothesis that the process that gives rise to the data can be described within the framework of probability theory. Only then, we are in the position that we can use probability theory to relate the mathematical model to the observed frequencies. Note the distinction between frequencies (observed facts) and probabilities (inferred knowledge). Of course, this is consistent with the fact that quantum theory does not describe the individual events themselves [3, 4].

Although probability theory provides a rigorous mathematical framework to make inferences, there are ample examples that illustrate how easy it is to make the wrong inference, also for mundane, every-day problems [33–36] that are not related to quantum mechanics at all. Subtle mistakes such as dropping some of the conditions [37], or mixing up the meaning of physical independence and logical independence, can give rise to all kinds of paradoxes [14].

In general, a computer simulation approach does not need the machinery of probability theory to relate simulation data to the experimental facts. A digital computer can generate the same kind of numbers as recorded in the experiment and there is no need to invoke inductive inference to make a comparison. Therefore, in a computer simulation, it should be possible to explain the facts without invoking "loopholes" or counter factual reasoning, for instance.

DOUBLE-SLIT MODEL

We focus on interference experiments with single-photons, leaving the case of massive particles for future research. As an example, we consider the double-slit experi-
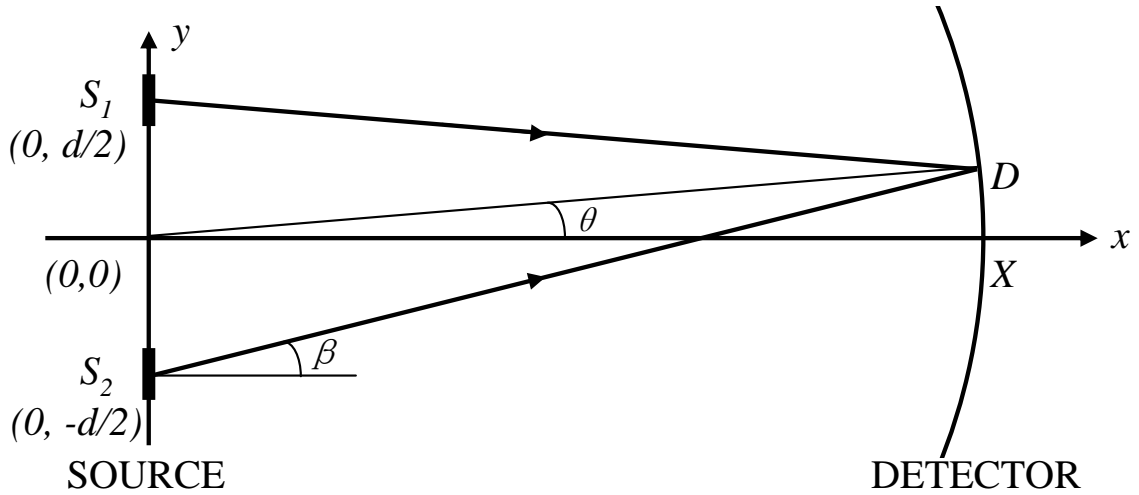
FIGURE 2. Schematic diagram of a simplified double-slit experiment with two sources S_1 and S_2 of width a, separated by a center-to-center distance d, emitting light according to a uniform current distribution (see Eq. (1)) and with a uniform angular distribution, β denoting the angle. The light is recorded by detectors D positioned on a semi-circle with radius X. The angular position of a detector is denoted by θ.

ments [38–40] in which the interference pattern is built up by recording individual clicks of the detectors.

Following Young [41] we can let the light impinge on a screen with two apertures and regard these apertures as the two virtual sources S_1 and S_2, see Fig. 2. For this system, a straightforward application of Maxwell's theory yields the intensity at the detection screen. If the sources S_1 and S_2 are lines of length a, separated by a center-to-center distance d (see Fig. 2), emit light according to a uniform current distribution, that is

$$J(x,y) = \delta(x)\left[\Theta(a/2 - |y - d/2|) + \Theta(a/2 - |y + d/2|)\right], \tag{1}$$

where $\Theta(.)$ denotes the unit step function. Then, in the Fraunhofer regime, the light intensity at the detector on a circular screen is given by [41]

$$I(\theta) = A\left(\frac{\sin\frac{qa\sin\theta}{2}}{\frac{qa\sin\theta}{2}}\right)^2 \cos^2\frac{qd\sin\theta}{2}, \tag{2}$$

where A is a constant, q is the wave number, and θ denotes the angular position of the detector D on the circular screen (see Fig. 2).

EVENT-BY-EVENT SIMULATION: GENERAL ASPECTS

The aim of this paper is to demonstrate that it is possible to use computer simulation as a scientific methodology to simulate (mimic) the build up of an interference pattern by single photons arriving one-by-one at a detector screen as observed a single-photon double-slit experiments without invoking concepts of wave theories.

The present paper builds on concepts developed in earlier work [42–54], demonstrating that it is possible to simulate quantum phenomena on the level of individual events without invoking concepts of quantum theory or probability theory. Specifically, we have demonstrated that locally-connected networks of processing units with a primitive learning capability can simulate event by event, the single-photon beam splitter and Mach-Zehnder interferometer experiments, Einstein-Podolsky-Rosen-Bohm (EPRB) experiments with photons, quantum cryptography protocols, universal quantum computation, Wheeler's delayed choice experiment, quantum eraser and Hanbury Brown-Twiss experiments. These particle-based simulation models can produce interference patterns even though the individual particles never directly communicate with each other, the only communication being indirectly through the interaction with the various devices used in the experiment such as polarizers, beam splitters and so on. For the cases studied earlier [42–54] it was sufficient to consider the detector as a passive device that simply registers the arrival of a particle.

The simple, passive detector model fails to reproduce the interference patterns of double-slit interference experiments in which there are sources and detectors only, as in Fig. 2. This can be seen as follows. Accepting the viewpoint that individual particles build up the interference pattern one by one and excluding the possibility that there is direct communication between the particles, by simply looking at Fig. 2, we arrive at the logically unescapable conclusion that the fact that we observe individual events that form an interference pattern can only be due to the presence and internal operation of the detector: There is nothing else that can cause the interference pattern to appear. The event-based model for the detector described in this paper is capable of reproducing these interference patterns. Incorporating these detector models in the simulation models of our earlier work does not change the conclusions of Refs. [42–53]. In this sense, the detector model adds a fully compatible component to our collection of event-by-event simulation algorithms.

SIMULATION MODEL

In our simulation model, every essential component of the laboratory experiment, that is the source and the detector array has a counterpart in the algorithm. The data is analyzed by counting detection events, just as in the laboratory experiment. The simulation model is solely based on experimental facts and trivially satisfies Einstein's criterion of local causality.

The simulation can best be viewed as a message-processing and message-passing process routing messengers through a network of units that processes messages. The processing units play the role of the components of the laboratory experiment and the network represents the complete experimental set-up. We now specify the operation of the basic components of the simulation model in full detail.

Messenger: In our simulation approach, we view each photon as a messenger carrying a message. Each messenger has its own internal clock, the hand of which rotates with frequency f. As the messenger travels from one position in space to another, the clock encodes the time of flight t modulo the period $1/f$. The message, the position of the clock's hand, is most conveniently represented by a two-dimensional unit vector

$\mathbf{e}_k = (e_{0,k}, e_{1,k}) = (\cos\phi_k, \sin\phi_k)$, where $\phi_k = 2\pi f t_k$ and the subscript $k > 0$ labels the successive messages. The messenger travels with a speed c/n where c denotes the speed of light in vacuum and n is the refractive index of the medium in which the messenger moves.

Source: In a simulation model in which the photons are viewed as messengers, the single-photon source is trivially realized by creating a messenger and waiting until its message has been processed by the detector before creating the next messenger. This ensures that there can be no direct communication between the messengers, implying that our simulation model (trivially) satisfies Einstein's criterion of local causality. The messengers leave the source at positions generated randomly according to the current distributions Eqs. (1). The distribution of the angle β is chosen to be uniform. When a messenger is created, its internal clock time is set to zero.

Detector: An event-based model for the detector cannot be "derived" from quantum theory, simply because quantum theory has nothing to say about individual events [3]. Therefore, from the perspective of quantum theory, any model for the detector that operates on the level of single events must necessarily appear as "ad hoc". From general considerations based on Maxwell's theory (see Section), it follows that a minimal model for the single-photon detector should have memory and a threshold feature.

The processing unit that acts as a detector for individual messages consists of two stages. The first stage consist of a deterministic learning machine (DLM) that receives on its input channel the kth message represented by the two-dimensional vector $\mathbf{e}_k = (\cos\phi_k, \sin\phi_k)$. In its simplest form the DLM contains a single two-dimensional internal vector with Euclidean norm less or equal than one. We write $\mathbf{p}_k = (p_{0,k}, p_{1,k})$ to denote the value of this vector after the kth message has been received. Upon receipt of the kth message the internal vector is updated according to the rule

$$\mathbf{p}_k = \gamma\mathbf{p}_{k-1} + (1-\gamma)\mathbf{e}_k, \tag{3}$$

where $0 < \gamma < 1$ and $k > 0$. Obviously, if $\gamma \neq 0$, a machine that operates according to the update rule Eq. (3) has memory.

The second stage of the detector uses the information stored in the internal vector to decide whether or not to generate a click (threshold behavior). As a highly simplified model for the bistable character of the real photodetector or photographic plate, we let the machine generate a binary output signal S_k using the threshold function

$$S_k = \Theta(\mathbf{p}_k^2 - r_k), \tag{4}$$

where $\Theta(.)$ is the unit step function and $0 \leq r_k < 1$ is a uniform pseudo-random number. Note that in contrast to experiment, in a simulation, we could register both the $S_k = 0$ and $S_k = 1$ events such that the number of input messages equals the sum of the $S_k = 0$ and $S_k = 1$ detection events. Since in experiment it cannot be known whether a photon has gone undetected, we discard the information about the $S_k = 0$ detection events in our future analysis.

The total detector count is defined as

$$N = \sum_{j=1}^{k} S_j, \tag{5}$$

where k is the number of messages received. Thus, N counts the number of one's generated by the machine.

It can be proven that as $\gamma \to 1^-$, the internal vector $\mathbf{p}_k$ converges to the average of the messages $\mathbf{e}_1, \ldots, \mathbf{e}_k$. In general, the parameter γ controls the precision with which the machine defined by Eq. (3) learns the average of the sequence of messages $\mathbf{e}_1, \mathbf{e}_2, \ldots$ and also controls the pace at which new messages affect the internal state of the DLM [42]. The event-based detector model has barely enough memory to store the equivalent of one message. Thus, the model derives its power, not from storing a lot of data, but from the way it processes successive messages. Most importantly, the DLM does not need to keep track of the number k of messages that it receives, a number that we cannot assume to be known because in real experiments we can only count the clicks of the detector, not the photons that were not detected. A detector screen is just a collection of identical detectors and is modeled as such. Each detector has a predefined spatial window within which it accepts messages.

The event-based detector model should not be regarded as a realistic model for say, a photomultiplier or a photographic plate and the chemical process that renders the image. Our aim is to show that, in the spirit of Occam's razor, this very simple event-based model can produce interference patterns without making reference to the solution of a wave equation. Concerning the memory aspect, as our approach does not rely on concepts of probability theory, our detector model is very different from earlier work that considered the hypothesis that memory effects in the equipment, operating as a random dynamical system over the field of p-adic numbers, can lead to interference phenomena [55, 56]. Regarding the use of a threshold mechanism, it is intuitively clear that single-photon detectors must necessarily operate as a threshold device because they have to discriminate between no and one photon. The presence of a threshold may have far reaching implications. For instance, it has been shown that it may lead to apparent violations of the Bell inequalities observed in EPRB experiments with photons [57]. The model presented in this paper differs from models proposed earlier in that there is a simple, one-to-one relation between the equations describing the event-based model and the material equations in Maxwell's theory (see Section).

SIMULATION RESULTS: DOUBLE-SLIT EXPERIMENT

As a concrete example, we consider the two-slit experiment with sources that are slits of width $a = \lambda = 670$ nm, separated by a center-to-center distance $d = 5\lambda$, see Fig. 2. In Fig. 3, we present the simulation results for a source-detector distance $X = 0.05$ mm. When a messenger (photon) travels from the source at $(0, y)$ to the circular detector screen with radius X, it updates its own time of flight, or equivalently its angle ϕ. This time of flight is calculated according to geometrical optics [41]. More specifically, a messenger leaving the source at $(0, y)$ under an angle β (see Fig. 2) will hit the detector screen at a position determined by the angle θ given by $\sin \theta = z \cos^2 \beta + \sin \beta \sqrt{1 - z^2 \cos^2 \beta}$ where $z = y/X$ and $|z| < 1$. The distance traveled is then given by $s = X \sqrt{1 - 2z \sin \beta + z^2}$ and hence the message is determined by the angle $\phi = 2\pi f s/c$ where c is the speed of light. As the messenger hits a detector, the detector updates its internal vector and decides whether to output a zero or a one. This process is
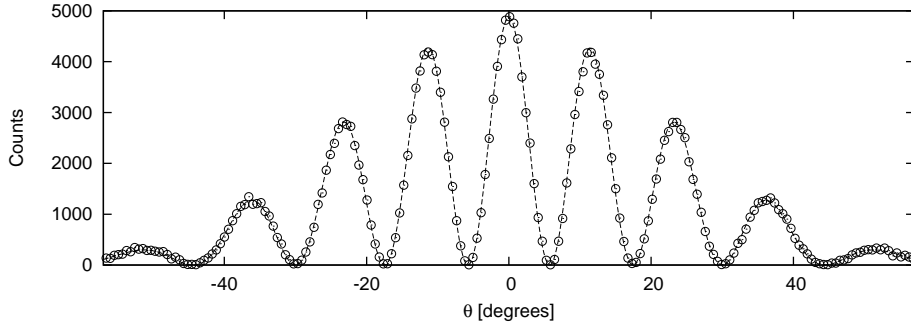
FIGURE 3. Detector counts as a function of the angular detector position θ as obtained from event-by-event simulations of the interference experiment shown in Fig. 2. The circles denote the event-based simulation results produced by the detector model defined in Section . The dashed lines are the results of wave theory (see Eq. (2)). The sources are slits of width $a = \lambda = 670$ nm, separated by a distance $d = 5\lambda$ and the source-detector distance $X = 0.05$ mm, see Fig. 2. The sources emit particles according to the current distribution Eq. (1).

repeated many times. The initial y-coordinate of the messenger is chosen randomly from a uniform distribution on the interval $[-d/2-a/2, -d/2+a/2] \cup [+d/2-a/2, +d/2+a/2]$. The angle β is a uniform pseudo-random number between $-\pi/2$ and $\pi/2$.

The markers in Fig. 3 show the event-by-event simulation results produced by the detector model described in Section with $\gamma = 0.999$. The result of wave theory, as given by the closed-form expression Eq. (2), is represented by the dashed line. From the mathematical analysis of the detector model, it follows that accurate results (relative to the predictions of quantum theory) are to be expected for γ close to one only. Taking for instance $\gamma = 0.99$ does not change the qualitative features although it changes the number of counts by small amounts (data not shown). From our simulation results, it is clear that without using any knowledge about the solution of a wave equation, the event-based simulation (markers) reproduces the results of wave theory.

An interactive Mathematica program of the event-based double-slit simulation which allows the user to change the model parameters and to verify that the simulation reproduces the results of wave theory may be downloaded from the Wolfram Demonstration Project website [58].

RELATION BETWEEN SIMULATION MODEL AND WAVE MECHANICS

Having demonstrated that the event-based model is capable of reproducing the results of wave theory without making recourse to the solution of the wave equation or even a single concept of wave theory, we now provide rigorous arguments that the event-based model contains the description that is given by Maxwell's theory.

From the definition of our model, it follows directly that the messenger can be viewed as the particle-based equivalent of a classical, linearly polarized electromagnetic wave with frequency f: The message $\mathbf{e}_k$ corresponds to a plane wave with wave vector $\mathbf{q}$ ($q = 2\pi f/c$). The time-of-flight t_k corresponds to the phase of the electric field. Adding

another clock to the messenger suffices to model the second electric field component orthogonal to the first one, and hence the fully polarized plane wave [52]. For the systems studied in the present paper including this extra feature, namely the equivalent of the polarization of the wave, is not necessary and therefore we confine the discussion to messages that are represented by two-dimensional unit vectors.

The internal vector $\mathbf{p}_k$ plays the role of the polarization vector $\mathbf{P}(t)$ of the detector material. Comparing the formal solution of Eq. (3)

$$\mathbf{p}_k = \gamma^k \mathbf{p}_0 + (1-\gamma) \sum_{j=0}^{k-1} \gamma^j \mathbf{e}_{k-j}, \tag{6}$$

with the constitutive equation

$$\mathbf{P}(t) = \int_0^t \chi(u)\mathbf{E}(t-u)du, \tag{7}$$

in Maxwell's theory [41], it is clear that both equations have the same mathematical structure: The left hand sides are convolutions of the incoming (applied) message (field) with memory kernel γ^j ($\chi(u)$) (in applications, we may assume that the initial value $\mathbf{p}_0 = 0$). Thus, the DLM is a simple model for the interaction of the individual photons with the material of the detector. The time-of-flight, corresponding to the phase of the electric field, is used to update the internal vector which corresponds to the polarization vector of the material.

This analogy can be carried much further: From the update rule Eq. (3), one can easily prove that if the time between the arrival of successive messages approaches zero and γ approaches one, the update equation turns into the constitutive equation of a Debye model in Maxwell's theory. Other models such as the Drude or Lorentz model can be derived in a similar manner. Operating in a certain, well-defined regime, the discrete model can be approximated by continuum equations that describe the coarse-grained behavior but the discrete models provide a description with details that can never be extracted from the corresponding continuum equations. Of course, the ultimate justification of the event-based model is that, as shown in Section , it can reproduce the results of wave theory.

CONCLUSION

We have demonstrated that it is possible to give a particle-only description for single-photon double-slit interference experiments. Our simulation model provides a simple, logically consistent, particle-based description of interference, does not require any knowledge about the solution of a wave equation, reproduces the results from wave theory, and satisfies Einstein's criterion of local causality.

We do not exclude that there are other event-by-event algorithms that reproduce the interference patterns of wave theory. For instance, in the case of the single-electron experiment with the biprism [5], it may suffice to have an adaptive machine handle the electron-biprim interaction. We leave this topic for future research.

Our simulation model makes specific predictions for the transient behavior of the distribution of events: They depend on the details of the model. However, the distribution that the model produces when it has reached the stationary regime agrees with wave theory and therefore, will be in concert with any experiment that reproduces the results of wave theory. Thus, a meaningful confrontation of our model with experiment requires that the latter has recorded all the events, starting with the very first photon that is detected (and not after alignment, calibration etc. has been performed). We hope that such time-resolved single-photon experiments will be performed in the near future.

ACKNOWLEDGMENT

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