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The Electrodynamic 2-Body Problem and the Origin of Quantum Mechanics

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We numerically solve the functional differential equations (FDEs) of 2-particle electrodynamics, using the full electrodynamic force obtained from the retarded Lienard–Wiechert potentials and the Lorentz force law. In contrast, the usual formulation uses only the Coulomb force (scalar potential), reducing the electrodynamic 2-body problem to a system of ordinary differential equations (ODEs). The ODE formulation is mathematically suspect since FDEs and ODEs are known to be incompatible; however, the Coulomb approximation to the full electrodynamic force has been believed to be adequate for physics. We can now test this long-standing belief by comparing the FDE solution with the ODE solution, in the historically interesting case of the classical hydrogen atom. The solutions differ. A key qualitative difference is that the full force involves a 'delay' torque. Our existing code is inadequate to calculate the detailed interaction of the delay torque with radiative damping. However, a symbolic calculation provides conditions under which the delay torque approximately balances (3rd order) radiative damping. Thus, further investigations are required, and it was prematurely concluded that radiative damping makes the classical hydrogen atom unstable. Solutions of FDEs naturally exhibit an infinite spectrum of discrete frequencies. The conclusion is that (a) the Coulomb force is not a valid approximation to the full electrodynamic force, so that (b) the n-body interaction needs to be reformulated in various current contexts such as molecular dynamics.

KEY WORDS: many-body problem; protein dynamics; functional differential equations; relativistic many-body problem; interpretation of quantum mechanics.

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1. INTRODUCTION

1.1. Aim

This author had earlier[1] proposed a new model of time evolution in physics using mixed-type functional differential equations (FDEs), with a tilt in the arrow of time. This paper sets aside the notion of a "tilt", and takes up only the FDEs of retarded electrodynamics. The retarded case already explicitly incorporates certain subtle mathematical features of electrodynamics and relativity noticed by Poincaré, but overlooked by Einstein and subsequent researchers. To bring out these subtleties, this paper reports on a numerically computed solution of FDEs of the 2-body problem of classical retarded electrodynamics.[2]

The use of the full (retarded) electrodynamic 2-particle force leads to the formulation of the electrodynamic 2-body problem as a system of FDEs that have *not* actually been solved earlier, numerically or otherwise, despite some sporadic attempts in simplified situations.[3] In the absence of a systematic way to solve these FDEs, a widely used alternative has been to approximate the full electrodynamic 2-particle force by the Coulomb force. This reformulates the electrodynamic 2-body problem as an easier system of ODEs, which can be numerically solved with exactly the same numerical techniques that are used for the ODEs of the classical 2-body problem of Newtonian gravitation. This alternative ODE formulation of the 2-particle electrodynamic interaction is incorporated, for example, in models of protein dynamics[4] underlying current software such as CHARMM, WASSER, AMBER, etc.

This alternative ODE formulation is, however, mathematically suspect, for it is known that solutions of FDEs may exhibit qualitative features impossible for solutions of ODEs. On the other hand, it is believed that, from the viewpoint of physics, the Coulomb force is an adequate approximation to the full electrodynamic force.

We can now put this long-standing belief to test: our numerical solution of the full-force FDEs enables us compare the two solutions in the historically interesting context of the classical hydrogen atom.

1.2. The Full Electrodynamic Force

In classical electrodynamics, the force between moving charges is given by the Lienard–Wiechert potentials combined with the Heaviside–Lorentz force law. The scalar and vector (retarded) Lienard–Wiechert potentials, are given by the expressions[5]

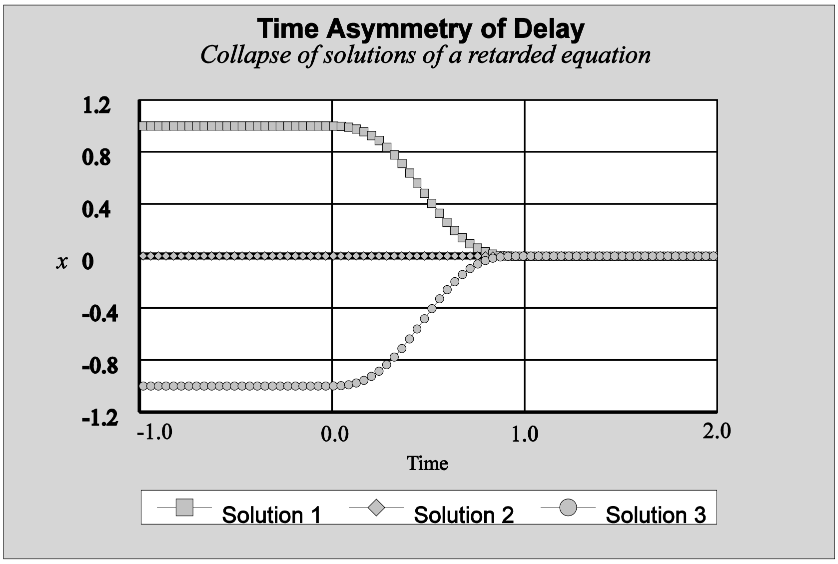

Fig. 1. The figure shows three different solutions of a retarded FDE $\dot{x}(t) = b(t)x(t-1)$, for a suitable choice of the function $b(t)$. Three different past histories prescribed for $t \leq 0$ lead to three different solutions all of which coincide for $t \geq 1$. Such a phase collapse is impossible with ODE where trajectories in phase space can never intersect. Because of this phase collapse, FDE, unlike ODE, cannot be solved backward, from prescribed future data.

Thus, on grounds of the known mathematical differences between FDEs and ODEs, it is reasonable to doubt, a priori, that the full electrodynamic force (6) can be validly approximated by the Coulomb force, by neglecting the vector potential.

A good way to settle this doubt is to put the matter to test by comparing the Coulomb-force solution with the solutions obtained using the full electrodynamic force. This requires a solution of the 2-body problem with the full electrodynamic force, and we accordingly proceed to calculate such a solution.

2. SOLVING FDES

2.1. Method 1

The mathematical features of FDEs briefly recapitulated above suggest that retarded electrodynamics involves a "paradigm shift" from "classical mechanics", for we now need past data rather than instantaneous

Need for past data as a paradigm shift.

data. In a debate on this question at Groningen, H. D. Zeh argued against any such paradigm shift. Zeh maintained that there was no need for past data, since data prescribed on a spacelike hypersurface (corresponding to an instant in spacetime) was adequate to solve the system of Maxwell's partial differential equations (PDEs) together with the Heaviside–Lorentz equations of motion for each particle.

The 1999 debate on the need for past data or a paradigm shift

Given all fields on a spacelike hypersurface, one can evolve them forward in time for a small region. *Given all fields*, in the vicinity of a single particle, its equations of motion reduce to a system of ODEs which can be solved in the usual way. We will call this method 1. We note that it implicitly involves the simultaneous solution of a *coupled* system of PDEs and ODEs.

2.2. Method 2

In contrast to method 1, the FDE formulation of the electrodynamic 2-body problem may be geometrically visualized as follows.[13] Assuming retarded potentials, the force on particle 1 at a given spacetime point $(a, 0)$ is evaluated as follows. One constructs the backward null cone with vertex at $(a, 0)$, and determines where it intersects the world line of particle 2, at a point (b, t), say (see Fig. 2). Given the world line of the particle 2 in a neighborhood of (b, t) one evaluates the resulting Lienard–Wiechert potential at $(a, 0)$, and uses this retarded potential to calculate the force on particle 1 at $(a, 0)$. This is the force given by (6). The force on particle 2 at any point is calculated similarly. Clearly, we can solve for the motion of either particle, only if we are given the appropriate portions of the *past* world line of the other particle. We will call this method 2.

2.3. Relating the two Methods

The Groningen debate brought out the following difficulty. *Both* the above methods seem to have the *same* underlying physical principles (Newton's laws of motion, possibly in a generalized form suitable for special relativity + Maxwell's equations). How, then, can these principles admit fundamentally incompatible interpretations of instantaneity and history-dependence?

2.4. The Need for Past Data

This issue can be readily resolved as follows. If retarded propagators (i.e., Green functions, or fundamental solutions of the wave equation, or retarded Lienard–Wiechert potentials) are assumed, then the field at any

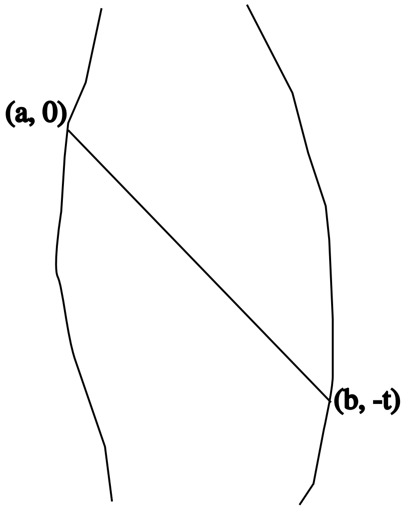

Fig. 2. To calculate the force acting on particle 1 at $(a, 0)$, one draws the backward null cone with vertex at $(a, 0)$. If this intersects the world line of the second particle at $(b, -t)$, one calculates the Leinard–Wiechert potential at $(a, 0)$, due to the motion of particle 2 at $(b, -t)$. Thus, determination of the present force on particle 1 requires a knowledge of the past motion of particle 2.

point x relates to particle movements in the past at the points x_a and x_b on the respective world lines of particles a and b, where the backward null cone from x respectively meets the world lines of the two particles (Fig. 3). Thus, to know the field at a point x we should know the particle world lines at and around the *past* points x_a, and x_b. If we do this for every point x on a spacelike hypersurface, the points x_a, and x_b will, in general, cover the entire past world lines of the two particles. Thus, in the 2-body context, given the assumption of retardation, prescribing the fields on a spacelike hypersurface is really equivalent to prescribing the *entire* past histories of the two particles. That is,

instantaneous data for e.m. fields = past data for world lines of particles

That is, the PDE + ODE method 1 only *hides* the underlying history-dependence of electrodynamics. (The above remarks need to be appropriately modified if, instead of assuming retardation, one assumes advanced or mixed-type propagators. For example, if we use advanced propagators, then ‘anticipation’ should be used in place of ‘history-dependence’, etc.)

2.5. FDE vs. ODE + PDE

While *both* methods require past data on the motion of the two particles, the intuitive schema underlying method 1 is currently inconvenient

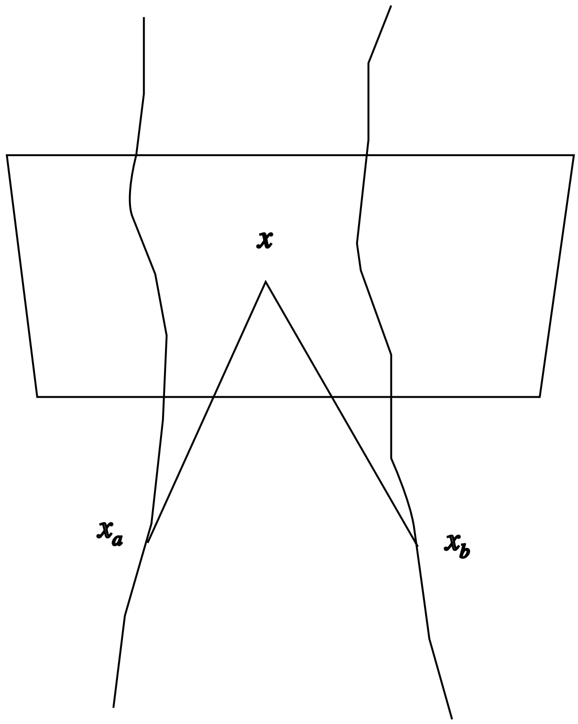

Fig. 3. Method 1 seems to requires only instantaneous data corresponding fields on a Cauchy hypersurface. Assuming only two particles and retarded propagators, the fields at any point x on the hypersurface relate to past particle motions at x_a and x_b. As x runs over the hypersurface, the points x_a and x_b will, in general, cover the entire past. Thus, in the retarded case, initial data for the fields is the same as past data for the world lines of the particles.

for the actual process of obtaining a solution. Formally speaking, there is no well-known existence and uniqueness theorem for a *coupled* system of PDEs + ODEs. [Separate existence theorems are, of course, known for PDEs (Maxwell's equations, in this case), and for ODEs (to which the particle equations of motion reduce, *if* all fields are given)]. Neither is there any well known numerical algorithm which converts the intuitive method of iteratively solving coupled PDEs + ODEs into an actual process of calculation.(14) Both formal proof and a numerical scheme can very likely be developed without much difficulty. However, neither is available as of now, so method 1 cannot, as of now, be used to obtain a solution of the full-force electrodynamic 2-body problem.

In contrast, for FDEs there is already a formal existence and uniqueness theorem from past data.[15] Further, there are well known numerical algorithms and tested computer programs available[16] (though they do not have all of the most desirable numerical characteristics, and the current code has not been formally proved to be error free). Accordingly, method 2 is currently the method of choice.

Incidentally, the PDE + ODE method 1 seems to need data on the *entire* past trajectories of the two particles. This is *more* information than is usually required for the FDE method 2. [Because of the numerical stiffness of the underlying equations, in practice, one is able to numerically solve the classical hydrogen atom with method 2 for only short time periods, of the order of a femto second (10^{-15} s), for which only a very short portion of the past history is needed.] That is, method 1, despite its appearance of preserving instantaneity and not needing any information from the past, actually seems to need *more* information about the past than method 2! A very careful analysis of the method would presumably show that the solution by method 1 actually uses information from only that part of the Cauchy hypersurface within the Cauchy horizon, so that information across the entire hypersurface is not needed, and the two methods are really equivalent. At present, however, that is still a conjecture.

3. SOLUTION OF THE ELECTRODYNAMIC 2-BODY PROBLEM

3.1. Prescription of Past History and Discontinuities

How should the past history of the two particles be prescribed? Existing physics provides no guidelines to help answer this question: exactly like fields on a spacelike hypersurface in method 1, it permits us to prescribe the past particle motions more or less arbitrarily.

Physical considerations for prescribing past data.

This has two consequences worthnoting. Thus, (1) mathematically, the past data for a FDE is *not* required to be a solution of the FDE, and (2) the mathematical theory of FDEs tells us that a discontinuity may well develop at the initial point where the prescribed past data joins with the solution of the FDE.

From a physical point of view, this past motion may be regarded as a bound or constrained motion—constrained, perhaps, by additional mechanical forces—and the discontinuity at the initial point may be attributed to the sudden removal of the additional constraint at $t = 0$. These discontinuities propagate downstream. While it is known from the general theory[17] that the discontinuities of a retarded FDE are typically smoothened out over time, i.e., that they move over to successively higher derivatives, we must recognize that the problem we are solving is (except in 1 dimension) technically a neutral[18] FDE (even though only retarded Lienard–Wiechert potentials are being used), so that no such smoothing need take place, and the discontinuities may persist.

The discontinuity creates a mathematical difficulty: for, in classical electrodynamics, the equations of motion are formulated assuming that the particle trajectories are at least thrice continuously differentiable (C^3). The numerical solution of the FDE by higher-order Runge–Kutta methods also assumes a similarly high level of smoothness, which assumption is not justified if the past history is prescribed arbitrarily.

This problem of discontinuities obviously is a suitable topic for further research, and in the sequel we shall set it aside and rely on the methods for handling discontinuities that are already incorporated into existing computer codes like RETARD and ARCHI [19], which handle discontinuities for example by switching to low-order polynomial extrapolation or predictor–corrector methods near a discontinuity. Both these programs are so written that they permit a discontinuity even in the function (positions, velocities) at the initial point, though we can always arrange initial conditions so that there is a discontinuity at most in the derivative (acceleration) at the initial point. We will prescribe past and initial data in such a way that discontinuities are confined to the acceleration and higher derivatives—though, like 'quantum jumps', it is not at present clear whether these are the only sorts of discontinuities that are 'physically acceptable'. The ARCHI program enables the tracking of such discontinuities, classified as 'hard' or 'soft' according to the theory of Willé and Baker.[20] Hard discontinuities are those that propagate instantaneously between components, while soft discontinuities are those that propagate over time. In the present context, since there are no advanced interactions, all discontinuities are soft, except for discontinuities between components (velocity, acceleration) representing derivatives. (Further, the ARCHI programme has certain refinements—such as the use of a cyclic queue to store past history—that are not immediately relevant.)

General strategy to prescribe past history.

3.2. The Classical Hydrogen Atom

To return to the physics, since our aim is to test how well the Coulomb force approximates the full electrodynamic force, let us consider the case of the classical hydrogen atom, without radiative damping. Suppose an electron and proton are for $t \leq 0$ constrained to rotate rigidly in a classical circular 2-body orbit, calculated using the Coulomb force. What will happen when this constraint is removed at $t = 0$? With the past history prescribed in this way, we now have a complete problem that can be solved by method 2.

The final prescription of past history, followed by a solution of the past value problem.

3.3. Equations of Motion

That is, we take the non-relativistic equations of motion to be given by the Heaviside–Lorentz force law for each particle:[21]

$$m\frac{d\mathbf{v}}{dt} = q\,(\mathbf{E} + \mathbf{v}\times\mathbf{B})\left[+\frac{2}{3}\frac{q^2}{4\pi\epsilon_0 c^3}\frac{d^2\mathbf{v}}{dt^2}\right]. \tag{14}$$

The radiative damping term given by square brackets in (14) has been dropped, since it is not immediately relevant to our purpose of deciding whether the electrodynamic force (6) can be approximated by the Coulomb force. (We know that, in the absence of radiation damping, with the Coulomb force, the initial "Keplerian" orbit should remain stable.) We also take the mass to be constant though, relativistically, only the proper mass is constant. This assumption, again, is appropriate to the comparison we wish to make between the Coulomb force and the full electrodynamic force.

3.4. Notation for the Explicit System of Equations

A slight change of notation is helpful for the explicit calculation. We let

$$\kappa = \frac{q_1 q_2}{4\pi\epsilon_0 m_1}, \quad \mu = \frac{m_1}{m_2}. \tag{15}$$

The mass ratio μ is dimensionless, while κ has dimensions of L^3T^{-2} (=length in units in which $c = 1$). Denote the 3-dimensional trajectories of the two particles by $\mathbf{r}_1(t)$, $\mathbf{r}_2(t)$. The delays τ, $\bar{\tau}$, and the vectors $\mathbf{R}_1$, $\mathbf{R}_2$ are defined by the simultaneous equations

$$c^2\tau^2 = R_1^2, \quad \mathbf{R}_1 = \mathbf{r}_2(t) - \mathbf{r}_1(t-\tau), \quad R_1 = ||\mathbf{R}_1||, \tag{16}$$

$$c^2\bar{\tau}^2 = R_2^2, \quad \mathbf{R}_2 = \mathbf{r}_1(t) - \mathbf{r}_2(t-\bar{\tau}), \quad R_2 = ||\mathbf{R}_2||. \tag{17}$$

Since here we consider only retarded solutions, for which $\tau, \bar{\tau} > 0$ we need to solve only the equations

$$R_1 - c\tau = 0, \tag{18}$$

$$R_2 - c\bar{\tau} = 0, \tag{19}$$

4.5. Discrete Spectrum and FDEs

Yet another argument for the relevance of FDEs to quantum mechanics.

The *discreteness* of the observed hydrogen spectrum has been regarded as another compelling argument against classical electrodynamics. Solutions of FDEs can, however, admit an infinite discrete spectrum.

Thus, for example, consider the *retarded harmonic oscillator*, given by the linear, second order, retarded FDE

$$\ddot{x}(t) = -x(t-1), \tag{50}$$

It is easy to see that a function of the form

$$x(t) = e^{z_k t}, \tag{51}$$

for complex z_k, is a solution of the Eq. (50) if and only if z_k is a solution of the*quasi*-polynomial equation

$$z^2 e^z = -1. \tag{52}$$

It is equally easy to see that the quasi-polynomial equation (52) has *infinitely many* complex solutions $z_k = x_k \pm i\, y_k$, and it is known(25) that the roots are discrete, with no cluster point, and that the large magnitude roots are given asymptotically by the approximate expression

$$y_k = 2k\pi + \epsilon_1(k), \tag{53}$$

$$x_k = -\ln y_k + \epsilon_2(k), \tag{54}$$

where $\epsilon_1(k) \to 0$, and $\epsilon_2(k) \to 0$ as $|z_k| \to \infty$.

(Had we dropped the retardation from (50), and applied the same procedure instead to the usual harmonic oscillator, given by the ODE $\ddot{x}(t) = -x(t)$, that would have led, in the well-known way, to a quadratic polynomial $z^2 = -1$ with exactly one pair of complex conjugate roots: i, and $-i$.)

Since the equation (50) is linear, any linear combination of these infinitely many oscillatory solutions of the form (51) is again a solution. Setting aside questions of convergence, it is clear that any *finite* linear combination of the form

$$x(t) = \sum_{k=1}^{n} a_k\, e^{z_k t}, \tag{55}$$

with z_k given by (54), say, is also a solution of (50). That is, in physical terms, the retarded harmonic oscillator, governed by the simple linear

FDE (50), exhibits an infinite spectrum of discrete frequencies. The general solution is a convergent linear combination of oscillations at an *infinity* of discrete ("quantized") frequencies. As in quantum mechanics, to determine a unique solution one needs to know an "initial" function. If the initial function is prescribed arbitrarily, we can expect discontinuities.

The above considerations remain valid for any linear FDE with constant coefficients and constant delay.(26) The locally linear approximation(27) suggests that such "quantization" is also to be expected for the non-linear FDEs of the electrodynamic 2-body problem. (For the FDE (12) this approximation may be obtained simply by replacing f by its first-order "Taylor" expansion, and then freezing the values of the delays t_r, in a neighborhood of the point at which we want to approximate the solution.)

Mere discreteness of the spectrum does not, of course, mean that the FDE formulation, using retarded electrodynamics, will correctly reproduce the actual spectrum of the hydrogen atom. Equally, mere discreteness of the spectrum was not an adequate argument *against* the classical hydrogen atom, which was prematurely rejected on the basis of the ODE formulation of the 2-body problem of electrodynamics. Though a further investigation of FDEs may still lead to a rejection of the classical hydrogen atom for the right reasons, it could, on the other hand, well help to clarify the "missing link" between classical and quantum mechanics, as in the structured-time interpretation of quantum mechanics.(28)

5. CONCLUSIONS

1. The Coulomb force is not a good approximation to the full electrodynamic force between moving charges.
2. The classical hydrogen atom was prematurely rejected on the basis of the ODE formulation of the electrodynamic 2-body problem.
3. The *n*-body problem involving electrodynamic interactions—as formulated, for example, in current software for molecular dynamics—needs to be reformulated using FDEs.

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