Numerical solutions in classical relativistic electrodynamics: one-dimensional bound positronium

1977 J. Phys. A: Math. Gen. 10 1097

(http://iopscience.iop.org/0305-4470/10/7/007)

J. Phys. A: Math. Gen., Vol. 10, No. 7, 1977. Printed in Great Britain.

Numerical solutions in classical relativistic electrodynamics: one-dimensional bound positronium

John C Kasher

Department of Physics, University of Nebraska at Omaha, Omaha, Nebraska 68101, USA

Received 22 March 1976, in final form 1 March 1977

Abstract. Two attractive charges of equal mass and charge magnitude are held a distance d apart for their entire past history, and at $t = 0$ are given a very small initial velocity away from one another. They slow down, stop, and fall into one another until they collide. We have used retarded fields and neglected radiation reaction in our Taylor series numerical solution, using constants to correspond to the $l = 0$, $n = 1$ orbit for positronium. The results are extremely close to the equivalent non-relativistic problem, thereby supporting the Schrödinger equation as a very good approximation to the true motion. We examine the Darwin approximation (supposedly correct to second order in β), and find it much closer to the non-relativistic solution than to the true relativistic one. The diameters of the various orbits and an upper limit to their corresponding periods are also suggested by the calculations.

1. The true relativistic solution†

1.1. Outline

Two attractive charges of equal mass and charge magnitude are held an initial distance d apart for their entire past history, and at $t = 0$ are given a very small initial velocity $v_0/c = \beta_0$ away from each other. They slow down, stop, then approach one another until they collide. Since the problem is relativistic, it takes a finite amount of time for each charge to 'see' a change in the motion of the other; hence for an initial time interval each moves in the electrostatic field of the other as seen in its original position. The problem is soluble analytically for this interval, and the results can be used to calculate the values of the various functions for the rest of the trajectory. We will treat the problem using the Lienard–Wiechert retarded fields, and will neglect any radiation-reaction force. The constants used in our calculations correspond to the $l = 0$, $n = 1$ orbit for positronium.

1.2. The analytic part of the trajectory

The energy equation governing a charge moving with an initial velocity in the electrostatic field of a fixed second charge is

$$m_0c^2 + m_0c^2\gamma_0 - q^2/d = m_0c^2 + m_0c^2\gamma - q^2/r \tag{1}$$

† When we use the term 'true' relativistic solution, we are merely contrasting it with the non-relativistic form, which is invalid when the charges are very close. It is certainly correct to say that our solution is not the true relativistic one in that we do not include radiation reaction; on the other hand, if we allow ourselves freedom to assume a built-in quantum condition that prevents radiation in order to stabilize the orbit of the positronium, then there is a certain validity in calling our solution the 'true' relativistic one.

where γ_0, $\gamma = 1/(1-\beta_0^2)^{1/2}$, $1/(1-\beta^2)^{1/2}$ and d is the initial separation. Since $\beta = dr/c\,dt$, the equation can be separated and integrated directly. If we define $D = q^2/m_0c^2d$ and use the restriction that $0 \leqslant (\gamma_0 - D)^2 < 1$ (which will be justified below) we arrive at

$$ct = \frac{d(\gamma_0 - D)}{(\gamma_0 - D)^2 - 1}\left(D^2 + 2\frac{Dr}{d}(\gamma_0 - D) + \frac{r^2}{d^2}[(\gamma_0 - D)^2 - 1]^{1/2} - (\gamma_0^2 - 1)^{1/2}\right)$$
$$- \frac{Dd}{[1-(\gamma_0 - D)^2]^{1/2}}\left\{\sin^{-1}\left[\left(\frac{(\gamma_0 - D)^2 - 1}{D}\right)\frac{r}{d} + \gamma_0 - D\right]\right.$$
$$\left. - \sin^{-1}\left(\frac{\gamma_0^2 - \gamma_0 D - 1}{D}\right)\right\}. \tag{2}$$

Thus r is an implicit function of the time. Equation (1) would then give us β, and successive differentiations of (1) would yield the higher-order derivatives in terms of β, r, or t.

To find out when this solution becomes invalid, and when we must begin using retarded fields, we set $ct = r$ in equation (2), since the change in the static field from one particle travels the distance r at speed c in reaching the second charge at time t.

To determine the relationship between γ_0 and D we equate the true energy at $t = 0$ (*not* that given by equation (1)) to the energies of the various Bohr orbits of two equal bound masses:

$$2m_0c^2\gamma_0 - 2m_0c^2 - q^2/d = -q^4 m_0/4\hbar^2 n^2$$

where n refers to the orbit. The equation can be written

$$\gamma_0 = 1 + D/2 - q^4/8c^2\hbar^2 n^2. \tag{3}$$

We find from our calculations that the larger our choice of γ_0 (and thus of β_0), the greater the percentage of the trajectory that is covered by the analytic solution. This is not desirable, since the analytic solution corresponds to a somewhat artificial physical situation. In reality, as the charges oscillate back and forth through one another they are governed completely by retarded fields (with the possible exception of the singularity at $r = 0$). So we want the analytic part to be minimal. This occurs when the end of the analytic region is as close as possible to where the charges stop before returning (in our calculations for positronium the retarded-field region comprises 99·999% of the distance travelled, and 99·5% of the elapsed time). The value of D from equation (3) that brings this about results in a value of $\gamma_0 - D$ that is just less than 1. This justifies using the restriction $0 \leqslant (\gamma_0 - D)^2 < 1$ mentioned above.

1.3. The retarded-field trajectory

The functions from the analytic portion can be used as retarded quantities in the Lienard–Wiechert force equation to find present-time functions in the first part of the retarded-field trajectory. These new values can then be used as retarded ones to calculate the next set of present-time functions, and so on. We have found it useful to define

$$y = [(1+\beta)/(1-\beta)]^{1/2}, \qquad z = R/c = (r + r')/c = t - t' \tag{4}$$

where the prime signifies retarded time, and r is measured from the point midway

between the charges. When this is done, the force equation

$$m_0 c\dot{\beta}/(1-\beta^2)^{3/2} = q^2(1+\beta')/R^2(1-\beta') \tag{5}$$

(where β is now defined as $-\mathrm{d}r/c\ \mathrm{d}t$) takes the form

$$\mathrm{d}y/\mathrm{d}t' = Dd(1+\beta')/cz^2. \tag{6}$$

If we realize that

$$\frac{\mathrm{d}t'}{\mathrm{d}t} = \frac{1+\beta}{1-\beta'}, \qquad \frac{\mathrm{d}z}{\mathrm{d}t'} = \frac{\mathrm{d}R}{c\ \mathrm{d}t'} = \frac{-(\beta+\beta')}{1+\beta} \tag{7}$$

then it is clear that any number of higher-order derivatives of y can be calculated with respect to t'. This suggests that we use as our numerical method a Taylor series expansion of y around t' to as many terms as are needed to obtain the desired accuracy. We used terms through the fifth derivative in our calculations.

The distance each charge is from the point midway between them can be calculated in similar fashion. Equations (7) and (5) can be used to find higher-order derivatives of z, which is then also expanded in a Taylor series to the desired accuracy around t'. Then from (4) the present position r is found. Higher-order derivatives of β can be calculated either from equation (5) or by differentiating it.

1.4. Considerations on numerical error

The Taylor series method is a very accurate one. In fact, most other methods attempt to achieve the same accuracy as a Taylor algorithm of a given order (Conte and de Boor 1965). We have used the method (Kasher 1976) in trajectory problems similar to the one presented here, and have obtained final values accurate to 0·00165%. (Of course, no such comparison can be made here, since the final values cannot be calculated analytically.)

The error factor is *beyond* all twelve significant figures used for *all* the calculations of r, and for the calculations for β up to $\beta = 0{\cdot}90$. From figure 2(*a*) one can see that the nature of the true velocity curve is clearly established by this value, and definitely separated from the Darwin and non-relativistic curve(s). The uncertainty for β is still in the twelfth figure past 0·95 for each new calculation, and barely reaches the eleventh figure at $\beta = 0{\cdot}99995$. Since less than 5×10^4 values of β (and position and acceleration) were obtained, we would expect that our calculations are quite accurate.

A built-in damping factor for propagation of error comes from the fact that as the number of calculations becomes larger the $\Delta t'$ used decreases. After the analytic solution $\Delta t'$ was determined by subtracting successive values of $t' = t - z$. Clearly, z decreases as time goes on. This damping factor helps considerably when the charges get very close. The higher-order derivatives become quite large; but since they are multiplied in the Taylor series by higher powers of a very small $\Delta t'$, they contribute very little to new calculations of β. This results in the very small error factor mentioned above.

We also varied the time interval to compare a number of successively rougher and finer calculations, and found that the solutions were quite stable below a certain maximum $\Delta t'$, and did not vary much as $\Delta t'$ was made smaller and smaller. We chose our $\Delta t'$ roughly one to two orders of magnitude below the maximum value, and did not use a finer one because the change in solutions was so slight.

2. The Darwin approximation

An approximate Lagrangian for interacting particles, correct to the order of v^2/c^2 inclusive, is (Jackson 1963)

$$L = -m_{01}c^2(1-v_1^2/c^2)^{1/2} - m_{02}c^2(1-v_2^2/c^2)^{1/2} + L_{\text{int}} \tag{8a}$$

with

$$L_{\text{int}} = \frac{q_1 q_2}{r_{12}}\left[-1 + \frac{1}{2c^2}\left(\boldsymbol{v}_1 \cdot \boldsymbol{v}_2 + \frac{(\boldsymbol{v}_1 \cdot \boldsymbol{r}_{12})(\boldsymbol{v}_2 \cdot \boldsymbol{r}_{12})}{r_{12}^2}\right)\right] \tag{8b}$$

where q_1, $\boldsymbol{v}_1$ and q_2, $\boldsymbol{v}_2$ refer to the two particles, and $\boldsymbol{r}_{12} = \boldsymbol{r}_1 - \boldsymbol{r}_2$. It is convenient to define the origin at the midpoint on the line joining the two charges. Since in our problem $q_1 = -q_2$ and $\boldsymbol{v}_1$ and $\boldsymbol{v}_2$ are antiparallel, the Lagrangian becomes

$$L = -m_0c^2\left(1-\frac{v_1^2}{c^2}\right)^{1/2} - m_0c^2\left(1-\frac{v_2^2}{c^2}\right)^{1/2} + \frac{q^2}{r_1+r_2}\left(1+\frac{v_1v_2}{c^2}\right) \tag{9}$$

which leads to the force equation

$$\frac{\dot{\beta}}{(1-\beta^2)^{3/2}} + \frac{\dot{\beta}q^2}{2m_0c^2r} = -\frac{q^2}{4m_0cr^2}(1-\beta^2). \tag{10}$$

In (10) we have taken advantage of the fact that $\dot{v}_2 = \dot{v}_1$, and $r_1 = r_2 \equiv r$. In our calculations we used the Taylor series method with equation (10) and its derivatives.

3. Results

3.1. Usefulness of the Darwin approximation

For perspective we include full-scale position, velocity, and acceleration curves in figure 1. The values of the true relativistic, Darwin, and non-relativistic solutions are so close on this scale that the curves are indistinguishable. To separate them we expand our time scale and focus on the last three per cent of the graphs (figures 2(*a*) and (*b*)). Now the true relativistic solution can be separated, but the Darwin and non-relativistic ones remain indistinguishable. In order to bring out more clearly the differences in the distance–time curves in figure 2(*a*) we extended our graph only down to 0·001 units of distance from the collision point. At this position the charges have reached a speed of only 0·08*c*; but the times for the two (three) curves are so close to the final collision times that the rest of each curve would be negligibly close to a straight line downward, and would provide no useful information. To see how each distance curve in figure 2(*a*) changes for smaller values of r we need only consult the velocity–time curves.

The three graphs in figure 2 indicate that the Darwin approximation is little better than the non-relativistic solution. To show this more clearly it is perhaps better to display the positions, velocities, and accelerations in tabular form. In table 1 we see that the Darwin approximation in each case is much closer to the non-relativistic values than to the true ones, suggesting that if an approximation is to be used the non-relativistic solution would be nearly as good as (and certainly much simpler than) the Darwin approximation.

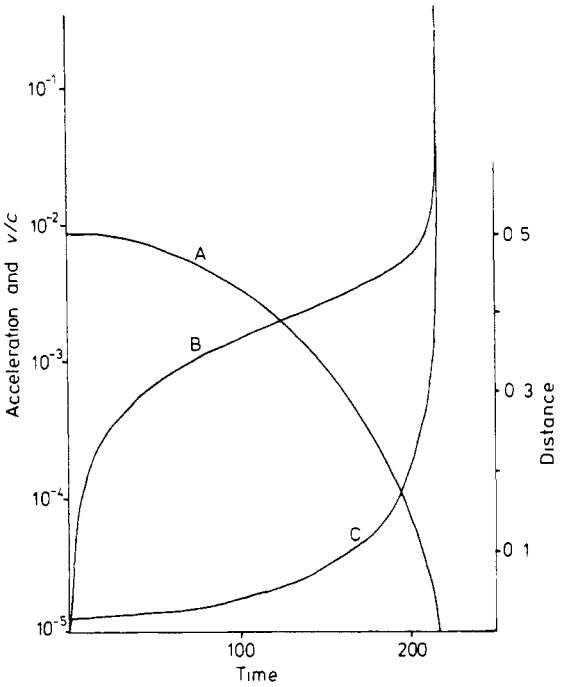

Figure 1. Full scale distance (A), velocity (B), and acceleration (C) against time. The true relativistic, Darwin, and non-relativistic curves are indistinguishable. (Distance is from the collision point, in terms of the initial separation.)

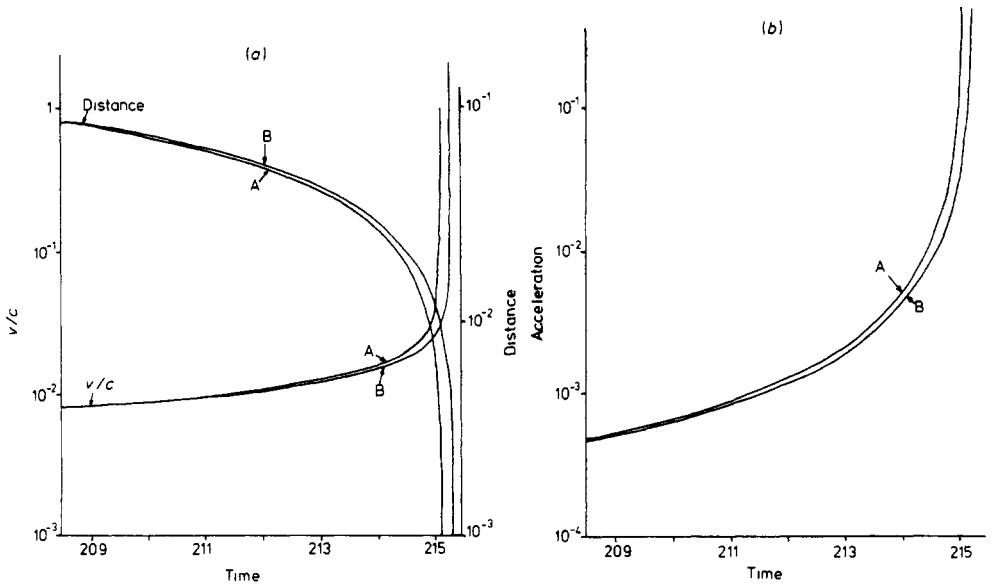

Figure 2. (*a*) Last 3% of the distance–time and velocity–time graphs. A, true curves; B, Darwin and non-relativistic curves. The Darwin and non-relativistic curves are indistinguishable. (Distance again from the collision point, in terms of the initial separation.)

(*b*) Last 3% of acceleration–time graph. A and B are the same as in (*a*). The Darwin and non-relativistic curves are again inseparable.

Table 1. Comparison of r, β, and $\dot{\beta}$ for the three solutions.

	r	β	$\dot{\beta}$	t
Non-relativistic	0·13175	$6{\cdot}100\times10^{-3}$	$1{\cdot}917\times10^{-4}$	
Darwin	0·13169	6·102	1·919	201·76
True relativistic	0·13070	6·130	1·948	
	5·77	$1{\cdot}010\times10^{-2}$	9·99	
	5·76	1·011	10·03	211·54
	5·60	1·027	10·62	
	1·45	2·110	$1{\cdot}58\times10^{-2}$	
	1·43	2·128	1·64	214·80
	1·06	2·473	2·94	
	$7{\cdot}68\times10^{-3}$	2·92	5·68	
	7·34	2·99	6·16	215·083
	$5{\cdot}86\times10^{-4}$	$1{\cdot}06\times10^{-1}$	$9{\cdot}36\times10^{0}$	
	$7{\cdot}55\times10^{-3}$	$2{\cdot}94\times10^{-2}$	$5{\cdot}87\times10^{-2}$	
	7·22	3·01	6·38	215·087
	$1{\cdot}78\times10^{-5}$	$5{\cdot}01\times10^{-1}$	$4{\cdot}95\times10^{3}$	
Non-relativistic	$6{\cdot}79\times10^{-3}$	$3{\cdot}11\times10^{-2}$	$7{\cdot}22\times10^{-2}$	215·122
Darwin	6·46	3·19	8·01	
	1·78	6·11	$1{\cdot}05\times10^{0}$	215·238
	1·06	7·93	3·08	
	1·31	7·11	1·93	215·2448
	$3{\cdot}87\times10^{-4}$	$1{\cdot}34\times10^{-1}$	29·13	
	$1{\cdot}15\times10^{-3}$	$7{\cdot}63\times10^{-2}$	2·63	215·2469
	$4{\cdot}8\times10^{-7}$	$9{\cdot}0\times10^{-1}$	1.04×10^{5}	

Collision times	
Non-relativistic	215·257
Darwin	215·247
True relativistic	215·087

3.2. Further comments on the true solution

In figure 3 we see that the relativistic acceleration does peak and come back down as β approaches one. Whether it approaches some finite limit as predicted as Huschilt *et al* (1973) is not clear. Our calculations are valid up to $\beta = 0{\cdot}99995$; but it appears that the slight oscillation of the acceleration around a limiting value would occur beyond this region, if it does occur. In any case, the limiting would be in the range of $1{\cdot}06\times10^{5}$ in natural units ($c/d = 1{\cdot}416\times10^{18}\,\mathrm{s}^{-1}$). This is considerably larger than the $2^{1/2}$ value obtained by Huschilt *et al.*

We have restricted ourselves to slightly more than half of a midpoint-to-midpoint oscillation because if we apply our approach to a very small initial separation and β_0 close to one the resulting analytic solution for the first part takes up far too much of the trajectory, and so the results would not correspond well to the real $l = 0$ orbit that we are considering. However, what we have calculated does give us an upper limit to the period of oscillation. When the charges approach one another, the retarded fields cause

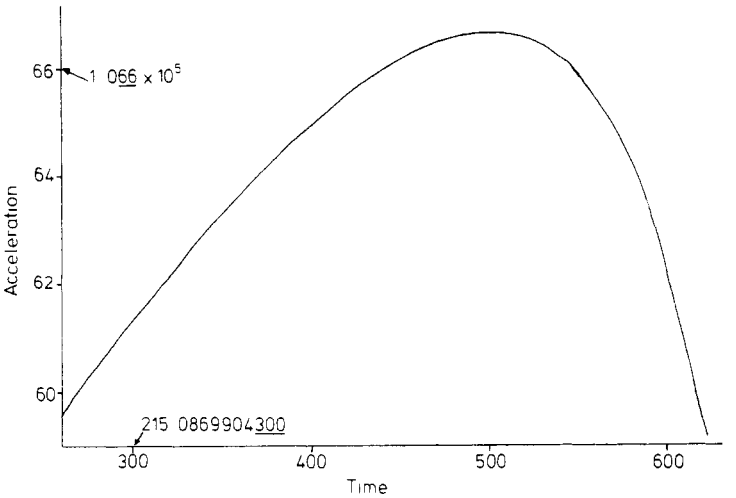

Figure 3. Final 10^{-8}% of acceleration–time graph. The acceleration turns down sharply as β approaches one as an upper limit.

them each to 'see' the other charge as being farther away than it actually is. When they are separating, however, they 'see' the other as being closer. Thus the effective force for the approaching charges is weaker than when they are separating; and it takes them a longer time to return from their largest separation than it does to travel out to it. So by quadrupling the return time we set an upper bound to the period of oscillation. For $l = 0$, $n = 1$ positronium the figure is

$$T < 6{\cdot}074476 \times 10^{-16}\ \text{s}.$$

We have run off values for parts of the paths of $n = 2$ and higher orbits (the computer time used makes full calculations like we did for $n = 1$ impractical), and the results strongly indicate that the following are the equations from which one can calculate the diameters and upper limits to the periods of the various orbits (n refers to the orbit):

$$\text{diameter} = n^2(2{\cdot}1166951 \pm 0{\cdot}0000141)10^{-8}\ \text{cm}$$

$$\text{period} < n^3(6{\cdot}074476 \times 10^{-16}\ \text{s}).$$

We also suspect that the tremendous increase in velocity at small distance that we found for the $n = 1$ orbit will occur for the higher orbits. In each case the graphs coincide exactly with the $n = 1$ results (except for the proper scale factor, of course) for as far as we carried out our calculations. Finally, our calculations suggest that the same type of results would follow for *any* $l = 0$ particle–antiparticle system, not just the electron–positron case.

Acknowledgments

We would like to thank Dr Charles Warden for helpful discussion on error analysis. This work was supported by the Senate Research Committee at the University of Nebraska at Omaha.

References

Conte S D and de Boor C 1965 *Elementary Numerical Analysis* 2nd edn (New York: McGraw-Hill)
Huschilt J, Baylis È E, Leiter D and Szamosi G 1973 *Phys. Rev.* D **7** 2844–50
Jackson J D 1963 *Classical Electrodynamics* (New York, London: Wiley)
Kasher J 1976 *Phys. Rev.* D **14** 939–44