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Relativistic dynamics of wave packets for spin-$\frac{1}{2}$ particles in an electromagnetic field

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Abstract. Classical and quantum dynamics of wave packets for spin-$\frac{1}{2}$ particles are analysed in the presence of an electromagnetic field. An almost exact agreement is found between these two approaches, both in the strong and the weak coupling limits. The question of negative energy states is discussed, and it is shown that they are not produced in such an interaction. The divergence problem of the perturbation expansion of the particles wavefunction is discussed, the source of which is explained.

1. Introduction

Recent study of the relativistic wave packets for a scalar particle [1] showed that under many circumstances classical theory gives an almost exact description of its dynamics in the electromagnetic field. This finding has an important value because it shows that classical theory can be used as an alternative to solving the problems of the particle's dynamics. Classical theory has certain advantages over quantum theory, such as it allows the use of classical concepts in modelling the particle's dynamics. Furthermore, classical theory is an initial value problem in contrast to quantum theory, which is both the initial and the boundary value problem. Very often the former is easier to solve and, therefore, can be used as an alternative to solving difficult scattering problems. However, in all these one should have a clear idea of what the limitations of classical theory are, and the study of this is the prime objective of this work.

In this work we analyse the classical and quantum dynamics of a wave packet for a spin-$\frac{1}{2}$ particle, which is interacting with the electromagnetic (EM) field. The basic idea in the classical study is to assume that the wavefunction represents the probability amplitude, i.e. its square modulus (for the spin-$\frac{1}{2}$ particles the square modulus must be taken in a broader sense) represents the probability density of finding a particle at a certain position. Likewise, the wavefunction in the momentum space represents the probability amplitude of a particle having certain momentum. Both these probability distributions can be used to determine the initial conditions for the classical trajectories, by generating random numbers which follow these distributions. After generating large numbers of classical trajectories, the classical probability distribution after time t is obtained by a suitable sampling [2]. The details of the procedure are explained in [2]. Based on this idea it will be shown that the scattering problem of a particle in the EM field is basically a classical process. The deviations which are noted are not significant and have simple explanations. The classical dynamics does not include the motion of the spin in the field, but despite this there is almost perfect agreement with the quantum results.

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Various aspects of dynamics of a particle in the EM field are discussed, and nearly exact agreement between the classical and the quantum analysis helps us in reaching certain conclusions. In particular this concerns the problem of the negative energy states, the problem of spin and the source of divergences in the perturbation expansion of the wavefunction.

2. Quantum theory

2.1. Solution of quantum equation

The basic relativistic quantum equations which describe interaction of a spin-$\frac{1}{2}$ particle with the EM field are†

$$\begin{aligned}\left(\hat{p}_0 - \frac{e}{c\hbar}A_0\right)\psi_b + \sigma\left(\hat{\boldsymbol{p}} - \frac{e}{c\hbar}\boldsymbol{A}\right)\psi_b &= \frac{mc}{\hbar}\psi_a \\ \left(\hat{p}_0 - \frac{e}{c\hbar}A_0\right)\psi_a - \sigma\left(\hat{\boldsymbol{p}} - \frac{e}{c\hbar}\boldsymbol{A}\right)\psi_a &= \frac{mc}{\hbar}\psi_b\end{aligned} \tag{1}$$

where $\sigma = \{\sigma_x, \sigma_y, \sigma_z\}$ are the spin-$\frac{1}{2}$ matrices (the fourth component is $\sigma_0 = \mathbf{I}$, where $\mathbf{I}$ is the unit matrix), and $A^\mu = \{A_0, \boldsymbol{A}\}$ are components of the four-potential. The four-momentum operator has the explicit form $\hat{p}^\mu = \{\hat{p}_0, \hat{\boldsymbol{p}}\} = i\{(\partial/c\partial t), -\nabla\}$. For the rest of this paper we shall use the standard, shorthand, notation. The contravariant vector x^μ has components $x^\mu = \{x_0, \boldsymbol{r}\}$, while the covariant has $x^\mu = \{x_0, -\boldsymbol{r}\}$. The invariant product of two vectors a^μ and b^μ is designated shortly $(ab) = a_\mu b^\mu$, so for example, the Lorentz condition for the four-potential, which we employ here, is

$$(\hat{p}A) = \hat{p}^\mu A_\mu = 0. \tag{2}$$

In this work it is assumed that the four-potential is a function of (xk), where $k = \{k_0 = w_0/c, \boldsymbol{k}\}$ is constant and represents the four-wave vector of the EM field. This assumption is not very restrictive since it covers wide ranging EM fields which are often used in the analysis of the interaction of radiation with matter. It covers a particularly interesting case of the plane wave EM fields which will be studied here. The number of parameters in (1) is unnecessarily large and can be reduced by a convenient scaling. The four-position vector $x = \{ct, \boldsymbol{r}\}$ is scaled by the Compton wavenumber of the particle $\kappa = mc/\hbar$, and in order to simplify the notation we use $\{t, \boldsymbol{r}\}$ to designate the four-vector $\{\kappa ct, \kappa \boldsymbol{r}\}$. The four-potential is written as $A = (E/k_0)\{a_0, \boldsymbol{a}\}$, where E is a constant which measures the amplitude of the vector potential. In the simplest case of the plane wave, where the vector potential $\boldsymbol{A}$ has a constant amplitude $\boldsymbol{A}_0$, it is defined by $E = k_0|\boldsymbol{A}_0|$ and plays the role of the maximal strength of the electric field in the interaction. Using these definitions the set (1) is now

$$\begin{aligned}(\hat{p}_0 - Qa_0)\psi_b + \sigma(\hat{\boldsymbol{p}} - Q\,\boldsymbol{a})\psi_b &= \psi_a \\ (\hat{p}_0 - Qa_0)\psi_a - \sigma(\hat{\boldsymbol{p}} - Q\,\boldsymbol{a})\psi_a &= \psi_b\end{aligned} \tag{3}$$

† This is the symmetrized form of the standard equations for the spin-$\frac{1}{2}$ particles. It is more convenient for practical analysis.

where $Q = eE/(mcw_0)$, and plays the role of the coupling parameter. In the last equation the four-momentum operator is also scaled with respect to Compton's wavenumber. The four potential a is now a function of the variable (kx), where $k = \{q, \boldsymbol{k}/\kappa\} = \{q, \boldsymbol{q}\}$ and $q = \hbar w_0/(mc^2)$.

The set of equations (1) has an analytic solution, which is briefly re-derived [3]. The two functions ψ_a and ψ_b are not independent of each other, and if ψ_a is given then

$$\psi_b = \sigma^\mu(\hat{p}_\mu - Qa_\mu)\psi_a. \tag{4}$$

The function ψ_a satisfies the second-order equation

$$(\hat{p}\hat{p})\psi_a + Q^2(aa)\psi_a - Q\Sigma'\psi_a - 2Q(a\hat{p})\psi_a = \psi_a \tag{5}$$

where

$$\Sigma' = \mathrm{i}\sigma^\mu\sigma^\nu k^\mu a'_\nu \tag{6}$$

with the property $\Sigma'\Sigma' = 0$. In the derivation of (5) we used the Lorentz condition (2), which in this case is $(ka') = 0$, where the prime designates the derivative with respect to the argument $u = (kx)$. The set (5) is solved by replacing ψ_a with

$$\psi_a = \mathrm{e}^{-\mathrm{i}(xp)}W(u) \tag{7}$$

where W satisfies the equation

$$W' = \frac{Q\Sigma' + 2Q(ap) - Q^2(aa)}{2\mathrm{i}(pk)}W \tag{8}$$

in the derivation of which we used $(pp) = 1$. The equation (8) has an analytic solution so that the most general ψ_a is

$$\psi_a = \left(\mathbf{I} + \frac{Q}{2\mathrm{i}(pk)}\Sigma\right)\mathrm{e}^{\mathrm{i}\eta}W_0 \tag{9}$$

where

$$\eta = -(px) - \int_{u_0}^{u} \mathrm{d}u' \frac{2Q(ap) - Q^2(aa)}{2(pk)} \tag{10}$$

and ψ_b is now given by

$$\psi_b = \left[(\sigma p) + \frac{Q}{2}\frac{(\sigma p)[\sigma k](\sigma a) - 2(\sigma a)(pk) + 2(\sigma k)(ap)}{(pk)}\right]\mathrm{e}^{\mathrm{i}\eta}W_0 \tag{11}$$

where $[\sigma k] = \sigma^\mu k^\mu$, and where the additional condition $(ka) = 0$ was used. The choice of u_0 and W_0 (which is a two-row matrix) depends on the initial conditions, which will be discussed later.

The solutions (9) and (11) are satisfied for two signs of p_0, i.e. for $p_0 = \pm\sqrt{1 + \boldsymbol{p}^2}$. The positive energy solutions $\psi_a^{(+)}$ and $\psi_b^{(+)}$ are defined for $p_0 > 0$, and the negative energy solutions $\psi_a^{(-)}$ and $\psi_b^{(-)}$ for $p_0 < 0$.

More convenient in further analysis is to use the linear combination

$$\phi = \psi_a + \psi_b \qquad \chi = \psi_a - \psi_b \tag{12}$$

and define the four-component wavefunction

$$\psi = \begin{pmatrix} \phi \\ \chi \end{pmatrix}. \tag{13}$$

Using this function, the most general solution which describes dynamics of a particle in the EM field is

$$\Phi = \int \mathrm{d}^3 p \left[\psi^{(+)} f(\boldsymbol{p}) + \psi^{(-)} g(\boldsymbol{p}) \right] \tag{14}$$

where f and g are scalar functions, which are determined from the initial conditions. At $t = 0$ it is assumed that there is no interaction between the field and the particle, i.e. the EM field is localized in the space region where the wavefunction of the particle is negligible. In other words, $a = 0$ at $t = 0$ in the region where Φ is defined, hence the initial ψ is

$$\psi_0 = \begin{pmatrix} [\mathrm{I} + (\sigma p)] W_0 \\ [\mathrm{I} - (\sigma p)] W_0 \end{pmatrix} \mathrm{e}^{\mathrm{i} \boldsymbol{p} \boldsymbol{r}} = \begin{pmatrix} \phi_0 \\ \chi_0 \end{pmatrix} \mathrm{e}^{\mathrm{i} \boldsymbol{p} \boldsymbol{r}}. \tag{15}$$

The function W_0 is defined so that $\psi_0^+ \psi_0 = 1$ which gives

$$W_0 = \frac{1}{2\sqrt{2 p_0 (1 + p_0)}} \begin{pmatrix} w_1 (1 + p_0 + p_z) + w_2 (p_x - \mathrm{i} p_y) \\ w_2 (1 + p_0 - p_z) + w_1 (p_x + \mathrm{i} p_y) \end{pmatrix} \tag{16}$$

where $|w_1|^2 + |w_2|^2 = 1$. From now on we use (16) in the analysis of (14).

2.2. The choice of the initial conditions

There are three parameters which specify (14) uniquely. These parameters are f, g and w_1, defined in (14) and (16), respectively. First, we note that in general the state Φ contains both positive and negative energy components. There has been much discussion about the role of the negative energy states in the relativistic dynamics of particles, but despite the controversies which were brought about by these discussions, we will make the assumption that in the initial state Φ_0 there are no negative energy states. This choice implies $g(\boldsymbol{p}) = 0$, which puts a constraint on the initial components of Φ_0. Setting $t = 0$ in (14) we find

$$\begin{aligned} \Phi_0^{(1)}(\boldsymbol{r}) &= \int \mathrm{d}^3 p \left[\phi_0^{(+)} f(\boldsymbol{p}) + \phi_0^{(-)} g(\boldsymbol{p}) \right] \mathrm{e}^{\mathrm{i} \boldsymbol{r} \boldsymbol{p}} \\ \Phi_0^{(2)}(\boldsymbol{r}) &= \int \mathrm{d}^3 p \left[\chi_0^{(+)} f(\boldsymbol{p}) + \chi_0^{(-)} g(\boldsymbol{p}) \right] \mathrm{e}^{\mathrm{i} \boldsymbol{r} \boldsymbol{p}} \end{aligned} \tag{17}$$

where

$$\Phi_0 = \begin{pmatrix} \Phi_0^{(1)} \\ \Phi_0^{(2)} \end{pmatrix}. \tag{18}$$

The set of equations (17) determines f and g, and if $g = 0$ then the components $\Phi_0^{(1)}$ and $\Phi_0^{(2)}$ are inter-related through the integral equation

$$\Phi_0^{(2)}(\boldsymbol{r}) = \frac{1}{(2\pi)^3}\int \mathrm{d}^3 p\,[\mathbf{I} - (\sigma p)][\mathbf{I} + (\sigma p)]^{-1}\mathrm{e}^{\mathrm{i}\boldsymbol{r}\cdot\boldsymbol{p}}\int \mathrm{d}^3 r'\,\mathrm{e}^{-\mathrm{i}\boldsymbol{p}\cdot\boldsymbol{r}'}\Phi_0^{(1)}(\boldsymbol{r}') \tag{19}$$

and

$$\Phi_0^{(1)}(\boldsymbol{r}) = \int \mathrm{d}^3 p\,\phi_0^{(+)} f(\boldsymbol{p})\mathrm{e}^{\mathrm{i}\boldsymbol{r}\cdot\boldsymbol{p}} = \int \mathrm{d}^3 p\sqrt{\frac{1+p_0}{2p_0}} f(\boldsymbol{p})\mathrm{e}^{\mathrm{i}\boldsymbol{r}\cdot\boldsymbol{p}}\begin{pmatrix} w_1 \\ w_2 \end{pmatrix}. \tag{20}$$

If w_1 and w_2 are independent of $\boldsymbol{p}$ then $\Phi_0^{(1)}$ is parametrized as

$$\Phi_0^{(1)}(\boldsymbol{r}) = F(\boldsymbol{r})\begin{pmatrix} w_1 \\ w_2 \end{pmatrix} \tag{21}$$

where F is a scalar function. Therefore, by specifying w_1 and by selecting only the positive energy states in the initial conditions, the function F determines uniquely the time evolution of the state Φ. The function F is determined by putting forward another proposition. It is known that

$$\rho(\boldsymbol{r}) = \Phi^{+}(\boldsymbol{r})\,\Phi(\boldsymbol{r}) \tag{22}$$

is conserved and positive, and despite controversies associated with this function we assume that it represents the probability density. This assumption is not necessary but it will be crucial when making comparison with the classical dynamics of the same process.

Therefore, if $\rho(\boldsymbol{r})$ is assumed to be known then obtaining $F(\boldsymbol{r})$ is not a trivial task (for simplicity we assume that F is real, otherwise a much more elaborate discussion is needed if the phase of this function is to be recovered, which involves knowing the probability current). The reason is that $\Phi_0^{(2)}$ is related to $\Phi_0^{(1)}$ through an integral transform and it is not clear how the equation

$$\rho(\boldsymbol{r}) = \Phi_0^{(1)^+}\Phi_0^{(1)} + \Phi_0^{(2)^+}\Phi_0^{(2)} \tag{23}$$

can be solved for F. In our study we will assume that $F(\boldsymbol{r}) = \rho^{1/2}(\boldsymbol{r})$, which gives for the amplitude $f(\boldsymbol{p})$ in (20)

$$f(\boldsymbol{p}) = \frac{1}{(2\pi)^3}\sqrt{\frac{2p_0}{1+p_0}}\int \mathrm{d}^3 r\,\mathrm{e}^{-\mathrm{i}\boldsymbol{p}\cdot\boldsymbol{r}}\rho^{1/2}(\boldsymbol{r}). \tag{24}$$

Of course $f(\boldsymbol{p})$ will not reproduce $\rho(\boldsymbol{r})$ but will give its overall shape.

3. Classical theory

The classical equations of motion for a particle interacting with the EM field are

$$mc\ddot{u}_\mu = \frac{e}{c}\left[\frac{\partial A_\nu}{\partial x^\mu} - \frac{\partial A_\mu}{\partial x^\nu}\right]u^\nu \tag{25}$$

where the dot designates the derivative with respect to the proper time s and $u_\mu = \dot{x}_\mu$. If the scaling of the previous section is used then the equations take the following form

$$\dot{u}_\mu = Q\left[\frac{\partial a_\nu}{\partial x^\mu} - \frac{\partial a_\mu}{\partial x^\nu}\right]u^\nu \tag{26}$$

where Q was defined in (3). It is assumed that a_μ is a function of (xk), in which case the set of equations (26) can be solved by putting $(xk) = \alpha s$, where α is a constant which needs to be determined [4]. Using this replacement we find that

$$\frac{\partial a_\nu}{\partial x^\mu} = \frac{k_\mu}{\alpha}\dot{a}_\nu \tag{27}$$

and the set of equations (26) becomes

$$\dot{u}_\mu = \frac{Q}{\alpha}k_\mu \dot{a}_\nu u^\nu - Q\dot{a}_\mu \tag{28}$$

and when integrated gives

$$u_\mu = \frac{Q}{\alpha}k_\mu(au) - Qa_\mu + \frac{Q^2 k_\mu}{2\alpha}(aa) + c_\mu \tag{29}$$

where c_μ is a constant which is determined from the initial conditions. If at $t = 0$ there is no interaction between the particle and the field then $a = 0$, hence $c_\mu = u^0_\mu =$ *the initial proper velocity of the particle.* The set can be solved for the unknown u_μ giving

$$u_\mu = -Qa_\mu + u^0_\mu + \frac{Qk_\mu}{\alpha}(au^0) - \frac{Q^2 k_\mu}{2\alpha}(aa) \tag{30}$$

from which one obtains $\alpha = (u^0 k)$. When the set is integrated again the coordinates x_μ are

$$x_\mu = u^0_\mu s + Q\int_0^s \mathrm{d}s'\left[-a_\mu + \frac{k_\mu}{\alpha}(au^0) - \frac{Q}{2\alpha}k_\mu(aa)\right] + x^0_\mu \tag{31}$$

where x^0_μ are the initial coordinates.

It is of particular importance to relate the proper time s to the real time t, since all the dynamics is analysed in the latter. This relationship is obtained by specifying $\mu = 0$ in (31), hence

$$t = \frac{s}{\sqrt{1 - v_0^2}} + Q\int_0^s \mathrm{d}s'\left[-a_0 + \frac{q}{\alpha}(au^0) - \frac{Qq}{2\alpha}(aa)\right] \tag{32}$$

where v_0 is the initial velocity of the particle. It is assumed that at $s = 0$ the real time is $t = 0$.

A particularly interesting case is when a is an oscillatory function with the property $a_\mu(\alpha s + 2\pi) = a_\mu(\alpha s)$. The period of oscillations of the trajectory in real time is obtained from (32)

$$\Delta_t = \frac{\Delta_s}{\sqrt{1 - v_0^2}} - \frac{Q^2 q}{2\alpha}\int_s^{s+\Delta_s} \mathrm{d}s'\,(aa) \tag{33}$$

where $\Delta_s = 2\pi/\alpha$. If the average of (aa) over one period is $\overline{(aa)}$ then

$$\Delta_t = \frac{2\pi}{\alpha}\left[\frac{1}{\sqrt{1-v_0^2}} - \frac{Q^2 q}{2\alpha}\overline{(aa)}\right]. \tag{34}$$

During the same time the particle moves to a new position, which is calculated from (31), thus giving the average translation velocity

$$v_{av} = \left(\frac{v_0}{\sqrt{1-v_0^2}} - \frac{Q^2}{2\alpha} q\,\overline{(aa)}\right) \Big/ \left(\frac{1}{\sqrt{1-v_0^2}} - \frac{Q^2 q}{2\alpha}\overline{(aa)}\right). \tag{35}$$

This result will be useful in the analysis of the dynamics of the particle in the oscillating EM field.

We will now describe the classical theory for the time evolution of the probability distributions [2]. The question which needs to be answered is the following: given the initial probability distributions of the particle's position and momentum, how do these distributions develop in time? It is exactly this question which is tackled in quantum theory, and one should try to answer it in classical theory.

Within the statistical interpretation of the wavefunction $|f(\boldsymbol{p})|^2$, where $f(\boldsymbol{p})$ was defined in (17), is interpreted as the probability density that a positive energy particle has momentum $\boldsymbol{p}$. Likewise (22) is interpreted as the probability density of a particle being at the position $\boldsymbol{r}$. By generating two sets of random numbers, one for the momentum and the other for the coordinates, which follow the distributions $|f(\boldsymbol{p})|^2$ and $\rho(\boldsymbol{r})$, respectively, we choose random initial conditions for the classical dynamics problem. For each set of conditions the trajectory is calculated from the equations (31). If N pairs of random initial conditions are chosen, then the final positions of these trajectories, after time t, will be spread over the space, which is assumed to be partitioned into the small volume elements δV. If n trajectories end in a volume element which encloses the coordinate $\boldsymbol{r}$, then the classical probability distribution $\rho(\boldsymbol{r}, t)$ is approximately given by

$$\rho(\boldsymbol{r}, t) \approx \frac{n}{N}\frac{1}{\delta V}. \tag{36}$$

It should be noted that the quantum probability distribution is given by (22), where the wavefunction is given by (14).

Throughout this paper it is assumed that $f(\boldsymbol{p})$ parametrizes as $\delta(p_x)\delta(p_y)f(p_z)$ which greatly simplifies the theory, but at the same time does not reduce the generality of the problem. Calculations with two typical probability distributions will be reported. One with

$$f(p) = \sqrt{\frac{d}{2\pi\sqrt{\pi}}}\,\mathrm{e}^{-p^2 d^2/2} \tag{37}$$

and produces the Gaussian-like shape of the probability distribution in the coordinate space. The other is

$$f(p) = \left(\frac{\mathrm{e}^{\alpha d} - 1}{\alpha[2(1-\mathrm{e}^{\alpha d}) + \alpha d(1+\mathrm{e}^{\alpha d})]}\right)^{1/2} \frac{1-\mathrm{e}^{-\mathrm{i}pd}}{2sh(p\pi/\alpha)} \tag{38}$$

which approximately produces the probability distribution

$$\rho^{1/2}(z) = \frac{C}{(1+\mathrm{e}^{-\alpha z})(1+\mathrm{e}^{\alpha(z-d)})}. \tag{39}$$

This shape has a nice feature that it is localized in the space $d > z > 0$, and in between it is nearly constant, which makes it particularly suitable for the study of the plane wave limit. Using the Gaussian-like shapes this is not easily achieved since that would mean pushing the EM field to $z \to \infty$ (it is assumed that at $t = 0$ there is no interaction between the EM field and the wave packet). In the case of (39) the EM field can be localized in the space $z < -|z_0| = z_0$ for $t < 0$, and by letting $d \to \infty$ the plane wave limit is achieved in the space $z \gg 1/\alpha$.

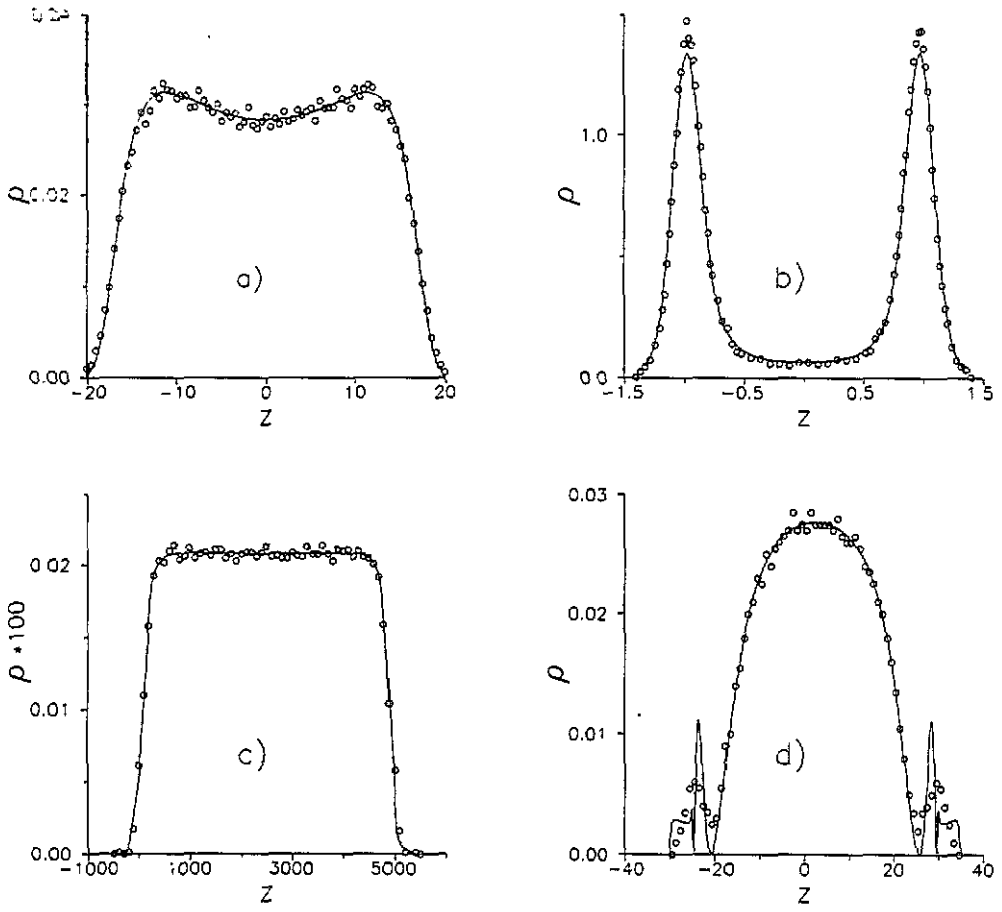

Figure 1. Classical (circles) and quantum (full curve) free probability distributions for the Gaussian-like, (*a*) and (*b*), and the rectangular-like shapes (*c*) and (*d*). The elapsed time for each of them is different and given in the text. (*a*) and (*c*) correspond to initially wide, and (*b*) and (*d*) to initially narrow, probability distributions.

As the preliminary test of how well classical theory reproduces the quantum dynamics, we have made several studies of the time evolution of free wave packets. Almost exact agreement between quantum and classical theory was found for the Gaussian-like shapes, independent of the initial conditions. Two typical cases are shown in figure 1. In the first (figure 1(*a*)) the initial wave packet is relatively broad ($d = 1$) compared to the Compton's wavelength, and in the second (figure 1(*b*)) it is narrow ($d = 0.1$). For the broad wave packet the time after which the comparison is made is $t = 20$ (time is measured in the

dimensionless units ct/κ, and in the real units that would be $t = 20\kappa/c$ s). The narrow wave packet is shown after $t = 1$. The classical results (circles) were obtained with 100 000 pairs of initial conditions. The agreement with the quantum results (full curve) is nearly exact (fluctuations of the classical results are due to the statistical spread of the random initial conditions), the agreement which was found in all the other circumstances.

The results for the rectangular-like shape (39) are shown in figure 1(*c*) and (*d*). Again, the same agreement was found as in the examples with the Gaussian-like shapes, except for very narrow wave packets. In fact, the most critical parameter is α, which measures the slope of the wave packet at the two ends. For a wide wave packet (figure 1(*c*)), with $\alpha = 0.01$ and $d = 5000$, after $t = 10000$ units of time, the agreement between the classical (circles) and the quantum (full curve) results is nearly exact. Figure 1(*d*) shows one example where the agreement is not so perfect, which is the result of the effect arising from the narrow edge of the wave packet ($\alpha = 10$, $d = 5$ and $t = 30$). However, these cases are rather isolated and should be avoided.

4. The limiting cases

Various examples of dynamics of the wave packets in the EM field were investigated. The EM field was assumed to be linearly polarized along the x axis, and it is described by the four-potential

$$a^\mu = \{0, \sin[q(z - t - z_0)], 0, 0\}\Theta(z_0 + t - z) \tag{40}$$

where $\Theta(\eta)$ is the step function meaning that the field at $t = 0$ is localized in the region $z < z_0$. The phase of the field (40) is chosen so that the requirement imposed in the classical equations of motion (at $t = 0$ the EM field is zero at the wave front) is fulfilled.

In all the cases investigated the agreement between classical and quantum results is almost exact. A few typical examples are reported, and in the first a Gaussian-like shape of the width $d = 1$ is investigated. The initial position of the EM wave front was taken at $z_0 = -10$, and the wavenumber of the field is $q = 1$, while the coupling parameter had the value $Q = 1$, which describes a moderately strong interaction. After $t = 100$ units of time the probability distribution is shown in figure 2(*a*). The classical results (circles) match almost exactly the quantum results (full curve). Another example is shown in figure 2(*b*) where the relevant parameters are: $z_0 = -10$, $q = 1$, $d = 0.1$, $Q = 5$ (strong coupling) and $t = 10$. In this example the EM wave front reached the point $z = 0$, so that the probability distribution for $z > 0$ is unaffected by the field. Such a good agreement between classical and quantum theory is not always found. Figure 2(*c*) shows an example for the rectangular-like probability distribution, with the following parameters: $z_0 = -100$, $d = 200$, $\alpha = 0.1$, $q = 0.1$, $Q = 1$ and $t = 500$. In figure 2(*d*) the parameters are the same except that $Q = 5$ (stronger interaction). It is interesting to note that in all the investigations the results are independent of the initial value for W_0, i.e. whatever the choice of w_1 the quantum and the classical ρ do not change.

Two extremes will be discussed in more detail: the weak and the strong interaction, because they give an interesting insight into the nature of the particle–EM field interaction.

4.1. The weak coupling limit

The weak coupling limit is defined for $Q \ll 1$, in which case the powers of Q higher than the first can be neglected. The wavefunction (13) is then approximately

$$\psi \approx \left[A + Q(a^\mu B_\mu) + Q\left(C_\mu \int_{u_0}^{u} a^\mu\right)\right] e^{-i(px)} \tag{41}$$

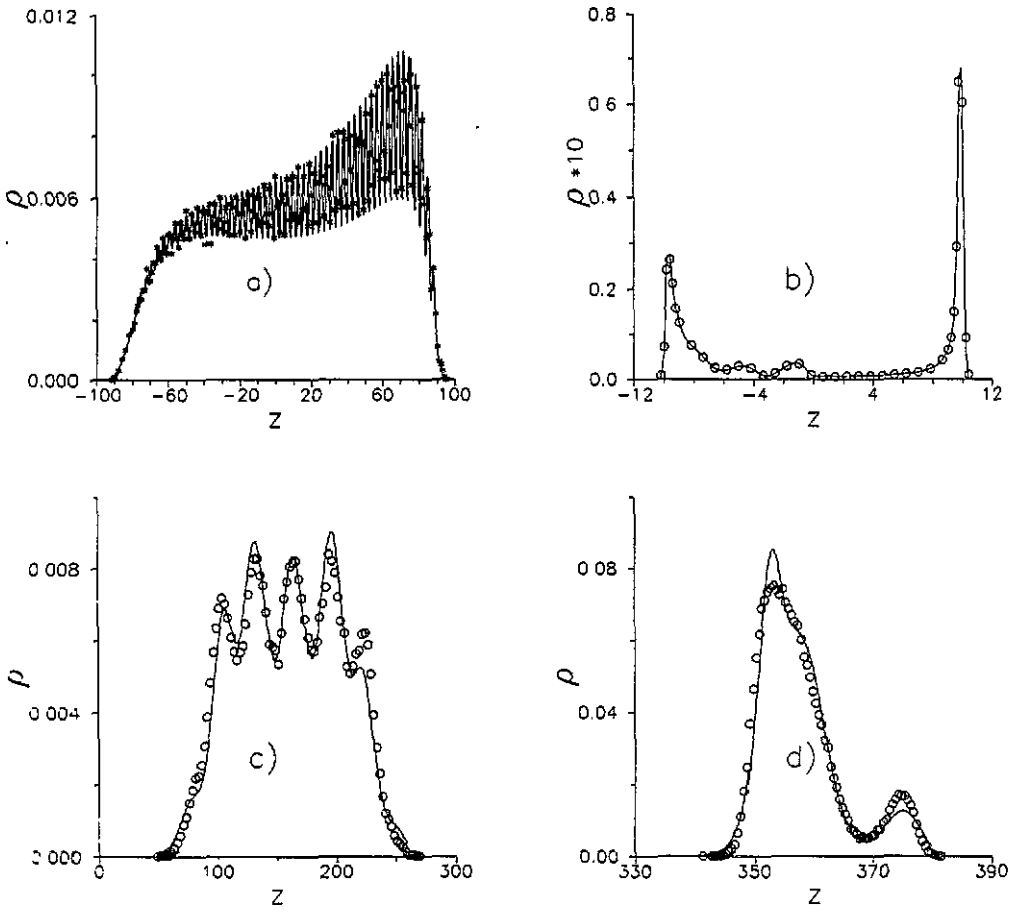

Figure 2. Classical (circles and crosses) and quantum (full curve) dynamics of the probability distributions under various circumstances. Gaussian-like shapes: (*a*) Moderately strong coupling and high-frequency field. (*b*) Strong coupling and initially narrow probability distribution. Rectangular-like probability distributions: (*c*) Moderately strong and (*d*) strong coupling limits.

where A, B_μ and C_μ are the four-column matrices, and are functions of p. The time evolution of the wave packet is now given by

$$\Phi = \int \mathrm{d}^3 p\, f(\boldsymbol{p}) \left[A(\boldsymbol{p}) + Q(aB(\boldsymbol{p}))Q\left(C(\boldsymbol{p}) \int_{\mu_0}^{u} a \right) \right] \mathrm{e}^{\mathrm{i}\boldsymbol{p}\boldsymbol{r} - \mathrm{i}p_0 t} \tag{42}$$

which has two components: one representing the time evolution of the free wave packet (the term with A) and the other representing the 'scattered' wave packet (the term with B). However, the latter has exactly the same form as the one for a free wave packet, except the 'modulation' term a is present. The functional dependence of B on p is of a similar form to A meaning that the second term in (42) represents the free-like movement of the wave packet. Therefore, in the weak coupling limit the motion of the free wave packet is not affected by the field except that its shape is modulated, which arises from a. These 'ripples' are difficult to observe since the free wave packet dominates the dynamics of the probability distribution. However, by calculating the difference $\rho - \rho_{\mathrm{free}}$ one eliminates the dominant term and only the contribution from the interaction is observed. In quantum

theory this difference is approximately

$$\rho - \rho_{\text{free}} = \Phi^{+}\Phi - \Phi^{+}_{\text{free}}\Phi_{\text{free}}$$
$$\approx Qa^{\mu} \int\int \mathrm{d}^3p\,\mathrm{d}^3p'\, f^{*}(p) f(p') \left[B^{+}_{\mu}(p)A(p') + A^{+}(p)B_{\mu}(p')\right]$$
$$\times \mathrm{e}^{\mathrm{i}r(p'-p)-\mathrm{i}t(p'_0-p_0)} \tag{43}$$

which consists of two parts, one of which involves integrals over the momentum space, and the other involves a^{μ}. The first part represents interference between the scattered and the non-scattered wave packets, and it is expected to be a quantum effect. Owing to the difference $p' - p$ in the exponential function, this contribution is a slowly oscillatory term. The term a^{μ} is the 'modulation' of the probability distribution and produces highly oscillatory 'ripples'.

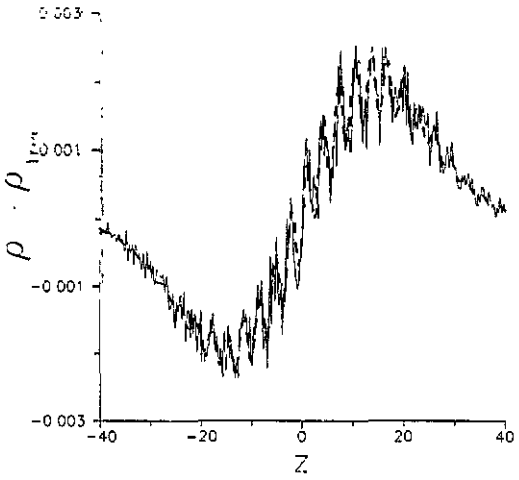

Figure 3. The difference between the interacting and the free probability distributions, in the weak coupling limit. The full curve represents classical calculations, and the broken curve the quantum ones. The initial shape is Gaussian-like.

Comparison with classical theory is difficult for practical reasons. In classical theory the probability distribution is obtained by generating random numbers, which have certain statistical fluctuations, and they should be smaller than the difference $\rho - \rho_{\text{free}}$. This is hard to achieve for a very small Q, so the comparison was made for $Q = 0.3$. The other parameters of the wave packet dynamics (for the Gaussian-like shape) were: $q = 1$, $d = 5$, $z_0 = -25$ and $t = 100$. Classical calculations were done with four sets of 10^6 pairs of random initial conditions, both for the free and the interacting probability distributions. Each set differed from the other by the initial seed. The results of subtracting the averages of the probability distributions are shown in figure 3 by the full curve. The broken curve shows the quantum results. The agreement between the two is nearly exact, within the statistical fluctuations. Therefore, even in this limit the dynamics of the particle in the EM field is basically classical, apart from the deviations associated with a particular choice of the initial wave packet.

It is interesting to investigate the limit which is often used in the quantum calculations: the plane wave limit of the particle's wavefunction. It is achieved by taking $d \to \infty$ in the shape (39) (omitting the normalization factor because the norm of such a wave packet is infinite) and take that part of the perturbed wave packet which is behind the wave front of the EM field (for $z < t + z_0$) and away from the origin ($z \gg 1/\alpha$). The amplitude $f(p)$ for such a wave packet is

$$f_\infty(p_z) = -\frac{2\mathrm{i}}{\alpha}\mathrm{P}\left[\frac{1}{sh(\pi p_z/\alpha)}\right] + \frac{1}{2}\delta(p_z) \tag{44}$$

where P[ ] stands for the principle value. It should be noted that owing to the parametrization of the amplitude f_∞ the average initial momentum of the particle is zero. If it is $\mathbf{p}^0$ then the 3D parametrization of $f(\mathbf{p})$ should be $\delta(p_x^0)\delta(p_y^0)f(p_z - p_z^0)$.

A typical integral which needs to be solved in the wavefunction, for this amplitude, is

$$I = \int \mathrm{d}p_z\, A(p_z) f_\infty(p_z) \mathrm{e}^{\mathrm{i}\eta(p_z)} \tag{45}$$

where $A(p_z)$ is a smooth function of p_z, and it has a square root branch point at $p_z = \pm\mathrm{i}$, the same as in $\eta(p_z)$. If f_∞ is replaced by (44) then

$$I = -\frac{\mathrm{i}}{4\alpha}\int_{-\infty}^{\infty} \mathrm{d}p_z\, A(p_z)\frac{\mathrm{e}^{\mathrm{i}\eta(p_z)} - \mathrm{e}^{\mathrm{i}\eta(-p_z)}}{sh(\pi p_z/\alpha)} + \frac{A(0)}{2}\mathrm{e}^{-\mathrm{i}t} \tag{46}$$

where for simplicity we have assumed that $A(p_z)$ is a symmetric function of p_z. In the weak coupling limit the integral becomes

$$I \approx -\frac{\mathrm{i}}{4\alpha}\int_{-\infty}^{\infty} \mathrm{d}p_z\, A(p_z)\frac{\mathrm{e}^{\mathrm{i}p_z z} - \mathrm{e}^{-\mathrm{i}p_z z}}{sh(\pi p_z/\alpha)}\mathrm{e}^{-\mathrm{i}p_0 t} + \frac{A(0)}{2}\mathrm{e}^{-\mathrm{i}t}. \tag{47}$$

The integration path can be distorted into the upper half of the p_z plane, at most to the point $p_z = \mathrm{i}$, where the integrand has the square root branch point. When z is sufficiently large, so that $\exp(-z) \ll 1$, then along this path the integral containing $\exp(\mathrm{i}p_z z)$ is negligible. The integrand containing $\exp(-\mathrm{i}p_z z)$ is not negligible, but this integration path can be distorted into the lower half of the p_z plane, where it is negligible. However, in doing this we must add the contributions from the residues, arising from the poles of $sh(z)^{-1}$. The dominant pole is at $p_z = 0$, while the next one is at $p_z = \alpha$. It can be shown that the integral is now

$$I = A(0)\mathrm{e}^{-\mathrm{i}t} + \mathrm{O}\left(\mathrm{e}^{-\alpha z}\right) \tag{48}$$

where the remainder comes from the contribution of the pole at $p_z = \alpha$. If $\alpha z \gg 1$ then the integral I is the plane wave limit. It should be noted that the initial momentum of the particle is $\mathbf{p}_{\mathrm{init}} = 0$, however, if it is $\mathbf{p}'$ then the limit (48) is proportional to $\exp(\mathrm{i}\mathbf{p}'\mathbf{r} - \mathrm{i}p_0' t)$. Therefore, the choice of the initial wave packet of the type (39) leads naturally to the plane wave limit, in the weak coupling case. Based on this result, it can be shown that the most general particle's wavefunction, in the plane wave limit, is

$$\Phi = A\,\mathrm{e}^{\mathrm{i}\mathbf{p}\mathbf{r} - \mathrm{i}p_0 t} + Q(aB)\mathrm{e}^{\mathrm{i}\mathbf{p}\mathbf{r} - \mathrm{i}p_0 t} \tag{49}$$

where the coefficients are obtained from (13) when the second and higher powers of Q are neglected. The first term represents the unperturbed particle's state, while the second is the perturbed one. In the language of quantum electrodynamics the second term represents contribution from a particle being scattered by the photon. In fact, based on this approximation the Klein–Nishina formula was derived [5].

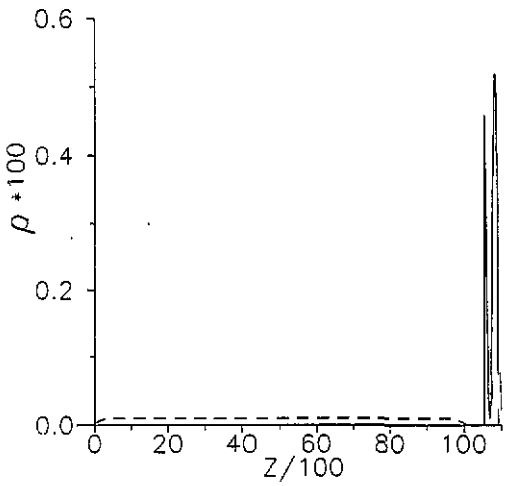

Figure 4. Very strong coupling dynamics of the rectangular-like initial shape (broken curve). After the wave front of the EM field has passed the initial wave packet all the probability is 'squeezed' into a narrow interval (full curve).

4.2. The strong coupling limit

The strong interaction between the EM field and the particle is characterized by $Q > 1$. In this case the dynamics of the wave packet cannot be based on the approximation where the plane wavefunction is represented by the series of various orders of corrections to the unperturbed wave, as was done in the weak coupling limit. In order to see this we repeat the derivation of the plane wave limit, but now for the entire wavefunction (13). The typical integral which needs to be solved is (46), but the phase is now

$$\eta(p_z) = p_z\left[z + \tfrac{1}{2}Q^2\,\overline{(aa)}\,(t - z + z_0)\right] + p_0\left[-t + \tfrac{1}{2}Q^2\,\overline{(aa)}\,(t - z + z_0)\right] \tag{50}$$

where the term of order Q is neglected. The integral along the path in the upper half of the p_z plane can be neglected provided the coefficient with p_z in (50) is positive, which is satisfied for

$$z > \frac{-\frac{1}{2}Q^2\,\overline{(aa)}\,(t + z_0)}{1 - \frac{1}{2}Q^2\,\overline{(aa)}} \tag{51}$$

and this gives the region where the plane wave approximation is valid. If we note that $\overline{(aa)} < 0$ and that the wave packet is unperturbed by the EM field for $z > t + z_0$, then the plane wave limit is valid in a small interval

$$(t + z_0) - \epsilon < z < t + z_0 \tag{52}$$

where

$$\epsilon = \frac{t + z_0}{1 - \frac{1}{2}Q^2\,\overline{(aa)}}. \tag{53}$$

Therefore, the perturbed part of the probability distribution, which is non-negligible, is confined to a narrow region of width ϵ, behind the front of the EM field. The rest of the affected probability distribution from $z = 0$ to $(t + z_0) - \epsilon$ is 'pushed' into this narrow interval, and because of the conservation of probability the average value of ρ in ϵ is

$$\overline{\rho} = 1 - \tfrac{1}{2}Q^2\overline{(aa)}. \tag{54}$$

Figure 4 shows one example of this dynamics, for a finite rectangular-like probability distribution, with the following parameters: $Q = 10$, $q = 0.01$, $d = 10\,000$, $\alpha = 100$ and $z_0 = -1000$. The initial probability distribution is shown by the broken curve, and after $t = 12\,000$ units of time it is shown by the full curve (it goes without saying that the classical theory reproduces the quantum results exactly). The unperturbed wave approximation, of the sort $\exp[-i(px)]$, is obviously not valid in the interval ϵ. However, a more general approximation $\Phi \approx \psi$ is valid, where ψ is given by (13) and $\overline{|\psi|} = \overline{\rho}^{1/2}$. Therefore, the modulus of ψ is a purely classical effect arising from setting the probability distribution into motion at uniform speed.

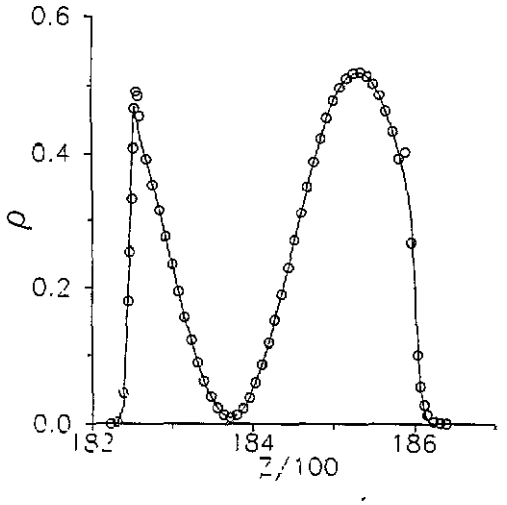

Figure 5. Test of the translation symmetry of the probability distribution in the strong coupling limit. When the probability distribution (full curve) is calculated at the time $t + \Delta_t$ and translated back by Δ (circles) the two match each other exactly.

The affected probability distribution moves at the average speed (35) and oscillates with the period (34), therefore, it has the following translation symmetry

$$\rho(\boldsymbol{r}, t) = \rho(\boldsymbol{r} - \boldsymbol{\Delta}, t + \Delta_t) \tag{55}$$

where $\boldsymbol{\Delta} = \boldsymbol{v}_{av}\Delta_t$. In our particular case, for the wave packet in figure 4, the period is $\Delta_t = 16\,336$ and $\Delta = 15\,708$. Two probability distributions were calculated at this time interval, and translated by the shift Δ. Figure 5 shows the result, where the full curve represents the probability distribution at $t = 20\,000$ and the circles at $t + \Delta_t$, but translated back by Δ. The two distributions match each other exactly, except for slight deviations at their edges, which might be caused by their dissipation during the time interval.

5. Discussion

Nearly exact agreement between the quantum and classical results for the dynamics of a spin-$\frac{1}{2}$ particle in the EM field raises several important questions. One, which comes first to our attention, is why classical theory, which does not take spin into account, reproduces

the quantum results for a spin-$\frac{1}{2}$ particle? If the particle has spin it would manifest itself in the quantum solution and the results would not be equal to the classical. The answer to this question needs much more elaborate discussion and will be reported separately [7]. In short, however, one can say that it can be shown that the spin of the particle is a classical concept, unlike the magnetic moment, which should be included in the classical equations of motion [8]. In fact, it follows from that discussion that the particles do not have the 'intrinsic motion' which gives rise to spin, instead one describes the manifestation of spin by the classical dynamics with point-like particles.

The second question which also comes immediately to our attention is why there is such a perfect agreement between classical and quantum theories when it is known that, according to the relativistic quantum dynamics, the negative energy states (antimatter) are created? The arguments in favour of the latter conclusion can be found in any text book on relativistic quantum theory. For example, Heitler says: 'An external field (if it varies sufficiently rapidly) can cause *transitions* from a state of positive energy to a state of negative energy' [9, p 111], or in Feynman's lecture notes on QED one finds an example where the transition probability to the negative energy state is calculated, not from QED but from relativistic quantum theory (the field is treated classically) [10, p 67]. Yet in our results no inconsistency between the classical and the quantum results is found, even for very high-frequency fields. It should be recalled that in classical theory only the positive energy states are included, and for real times no transition into the negative energy states is possible. In fact, we now show that in quantum theory such a transition is not possible, at least for the type of interaction which we discussed.

The time evolution of the wave packet, in the presence of the EM field is (14) (where $g = 0$), and in order to avoid any controversies, we assume that the incident EM wave has finite length, and that the components of the wave packet are analysed when this wave has passed, and is far away from the wave packet. Therefore, for large enough t

$$\Phi_\infty = \int \mathrm{d}^3 p\, \psi_\infty^{(+)} f(\boldsymbol{p}) \tag{56}$$

where ψ_∞ is given by (13) for $p_0 > 0$, and the components are given by (9) and (11). In these components the only quantity which is 'history dependent' is the phase η, since the others depend on the actual value of the field, which is assumed to be zero in the region of the wave packet. Therefore

$$\psi_\infty^{(+)} = \psi_0^{(+)} \exp\left[-\frac{\mathrm{i}}{2(pk)} \int_{u_0}^{u_1} \mathrm{d}u' \left(2Q(ap) - Q^2(aa)\right)\right] = \psi_0^{(+)} \mathrm{e}^{\mathrm{i}\eta_0} \tag{57}$$

where ψ_0 is given by (15). The value of u_1 is determined by the length of the EM field. The wave packet is now

$$\Phi_\infty = \int \mathrm{d}^3 p\, \psi_0^{(+)}(r, p) f(p) \mathrm{e}^{\mathrm{i}\eta_0(p)} \tag{58}$$

from which it is obtained that no negative energy states are present because

$$\int \mathrm{d}^3 r\, \psi_0^{(-)^+} \Phi_\infty = 0. \tag{59}$$

This result is in accordance with the classical study, where the agreement with the quantum results is achieved without including the negative energy states.

The conclusion is in direct disagreement with the aforementioned observations by Heitler and Feynman. We will not elaborate here the controversy since it involves a discussion which needs more space than is available. A separate report on the subject will be given [11], but here we will only mention that the issue of the creation of antimatter goes back to the basic development of quantum theory. It can be shown that some basic errors were made in reaching the conclusion that Dirac's equation, coupled to the external field, predicts creation of antiparticles (the negative energy states). This paper, on the examples which were demonstrated, supports such a conclusion.

There is another question which comes out from the analysis, but is not so self-evident. It concerns the exact solution (9) and (11) of the quantum equations of motion and its expansion into the perturbation series. The solution is one of the special cases among those possible from the basic quantum equations which describe interaction of the EM field with the spin-$\frac{1}{2}$ particle. The most general set of these equations is [12]

$$\begin{aligned} &[(\gamma\hat{p}) - 1]\psi = Q(\gamma a)\psi \\ &(\hat{p}\hat{p})\, a_\mu = 4\pi(\alpha/Q) j_\mu \end{aligned} \tag{60}$$

where α is the fine-structure constant and γ are the Dirac matrices. The first equation is the well known Dirac equation, and the second one is the equation for the EM field (its four-potential) in the presence of the current. The set of equations have a formal solution in the form of the set of integral equations [12, p 76]

$$\begin{aligned} \psi &= \psi_0 + Q \int \mathrm{d}^4x'\, S(x - x')(\gamma a(x'))\, \psi(x') \\ a_\mu &= a_\mu^0 + 4\pi \frac{\alpha}{Q} \int \mathrm{d}^4x'\, G(x - x')\, \psi^+ \gamma_\mu\, \psi \end{aligned} \tag{61}$$

where we used the expression for the current $j_\mu = \psi^+\gamma_\mu\psi$. ψ_0 is the unperturbed wavefunction and a_μ^0 is the unperturbed four-potential. The coupled set of equations is nonlinear and obviously not easy to solve. If a_μ is replaced in ψ then the particle's wavefunction is

$$\begin{aligned} \psi = \psi_0 &+ Q \int \mathrm{d}^4x'\, S(x - x')(\gamma a^0)\psi \\ &+ 4\pi\alpha \int \mathrm{d}^4x'\, S(x - x') \int \mathrm{d}^4x''\, G(x' - x'')\gamma^\mu(\psi^+\gamma_\mu\psi)\, \psi \end{aligned} \tag{62}$$

and one way to solve it is by iteration. However, there is a hidden danger in this procedure which we want to mention. The terms with α are interpreted as the radiative corrections when the probability distribution is affected by its self-produced EM field. We will neglect this effect and hence all the terms with α. In this case the set of equations (60) has an exact solution and it is given by (9) and (11). On the other hand, the integral equation (62) can be iterated to produce the solution, which is a series in powers of Q, and in principle should be equal to the exact solution. By comparing the two solutions we might find the answer to the source of the infinities which are found in the series.

The expansion of (13) in powers of Q is relatively straightforward, but one encounters a serious problem. The terms of the form

$$\exp\left[\mathrm{i}\frac{Q^2}{2(pk)}\,\overline{(aa)}\,(u - u_0)\right] \tag{63}$$

appear in (13) and although Q might be small the expansion of this function might not have meaning if u is large. The contribution of these terms in the expansion of ψ start with Q^2, and the leading coefficient which is not small in the limit $|u| \gg 1$ is

$$\psi^{(2)} \approx A u \mathrm{e}^{-\mathrm{i}(px)}. \tag{64}$$

However, it should be recalled that in order to find the scattering amplitudes for various processes one takes the Fourier transform of the coefficients in the expansion, e.g. [12, equation 18.13]. The second-order scattering amplitude in this case is

$$I^{(2)} = \int \mathrm{d}^4x \, \mathrm{e}^{\mathrm{i}(p'x)} \int \mathrm{d}^4x' \, S(x-x')(\gamma a^0) \int \mathrm{d}^4x'' \, S(x'-x'')(\gamma a^0)\psi_0 \tag{65}$$

which gives the contribution from $\boldsymbol{p}' - \boldsymbol{p} = \pm 2\boldsymbol{q}$ and $\boldsymbol{p}' = \boldsymbol{p}$. The last contribution is infinite and its source is easily explained from (64), the Fourier transform of which is

$$\int \mathrm{d}^4x \, \mathrm{e}^{\mathrm{i}(px')} u \mathrm{e}^{-\mathrm{i}(px)} \tag{66}$$

which is indeed infinite for $p = p'$ (one should recall that without u in (66) this would be the definition of the Dirac function, which is not considered infinite). Therefore, the source of the infinity in the expansion of the scattering amplitude is basically the wrong way one solves the set of equations (60). It is assumed that one can start from the unperturbed waves ψ_0 and build up the solution by iteration, however, this is not true because even for a very small Q the exponent in (63) can be large because u is large (in the Fourier transform $-\infty < u < \infty$). The source of infinities in the power series in α is of the same nature. This is because the kernel $S(x-x')$ carries the information about the expansion of the exact solution in the powers of Q, which in fact is not possible in the infinite interval of u. There are two ways one can get around these difficulties. One way is to use the exact solution (13) for ψ_0 in the set of equations (61). The kernel $S(x-x')$ becomes more complicated, but it can be found since the exact solutions ψ_0 are known. The other way is to note that all the infinite terms contribute to the expansion of the function (63), and since this function contributes only the phase to the wavefunction, the transition probabilities are independent of it. Therefore by simply neglecting the infinite contributions in the expansion (62) one does not affect the cross sections. However, one may make it more formal by adding and subtracting terms in the Dirac equation: one going into the mass term, called the experimental mass, and the other into the four-potential. The four-potential is modified in such a way so that $\overline{(aa)} = 0$, in which case the infinite terms disappear. Such a modification of the four-potential is possible because of the gauge invariance of the potential.

Nearly perfect agreement between the classical and quantum results could be the result of the 1D assumption made in section 3. However, this assumption is only superficially 1D since we still solve the 3D equations, however, by assuming that the initial probability distribution is delocalized in the x and y directions and localized in the z direction. In this respect the problem which is being solved is more general than most of the problems in the QED, since there the initial state of electron is entirely delocalized. However, it would indeed be of interest to see what the comparison is like when the initial probability is localized in all directions. The analysis of the spin [7], where the localization of the probability distribution is in 2D, supports the view that similar agreement may be found in this more general case.

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