Angular momentum of a relativistic wave packet

P. Strange*
School of Physical Science, University of Kent, Canterbury, Kent CT2 7NH, United Kingdom
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Quantum-mechanical spin is often thought of in terms of classical angular momentum. In fact spin is defined by its commutation relations and the spin and orbital angular momentum operators are very different. Here we solve the Dirac equation in a rotating frame of reference and create a localized wave packet from the resulting wave functions to examine the consequences of the rotational motion. We highlight some unexpected effects in the properties of the wave packet and show that the spin operator and orbital angular momentum operator describe different aspects of the rotational properties of the wave packet. It is also observed that neither quantum-mechanical spin nor orbital angular momentum can be fully understood within an inertial frame.

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I. INTRODUCTION

Angular momentum is a fundamental quantity in quantum theory. It forms the basis of much of our understanding of atoms, molecules, and materials and is key to the interpretation of many spectroscopies. Frequently there are spin and orbital contributions to the total angular momentum which is conserved. While orbital angular momentum is generally thought of as a quantum analog of the classical angular momentum, the physical manifestation spin is determined by the mathematical properties and commutation relations of its operators.

Spin was postulated by Uhlenbeck and Goudsmit [1] as a self-rotation of a particle, which they considered as a charged sphere, to explain doublets seen in atomic spectra. Its quantum nature was later verified in the Stern-Gerlach experiment [2]. This view of spin is now known to be unacceptable because the speed of rotation required to produce the known electron magnetic moment is much greater than the speed of light [3]. However the spin operator does obey nonrelativistic angular momentum commutation relations which has led to a number of researchers putting forward models of spin based on the classical notion of rotation [4,5]. Spin does not arise naturally in nonrelativistic quantum mechanics; it was introduced phenomenologically by Pauli into nonrelativistic quantum theory. His approach turned out to be the nonrelativistic limit of relativistic quantum theory. This has been investigated by a number of authors [8,9]. In particular, Galindo and Sanchez Del Rio [9] have shown that the magnetic moment of the electron drops out of a linearized version of the nonrelativistic Schrodinger equation in the same way as it does from the Dirac equation. However, as stated by Kudryashova and Obukhov [5], “the true understanding of spin as an essentially quantum property of matter is achieved only through quantum theory.” As spin only arises naturally in relativistic theory, this really refers to relativistic quantum mechanics.

In a number of papers recently spin and orbital angular momentum have been discussed, particularly in the context of the structure of vortices in relativistic wave packets [10,11]. The underlying view of spin has been that it takes on many of the properties of a classical rotation. Indeed this is borne out by the work of Chuu et al. [12] where a Gaussian wave packet was set up and the current density was shown to be a vector rotating about its center. Our purpose in this paper is to address the question of how similar quantum-mechanical spin and orbital angular momenta are and how they relate to our classical notions of these quantities. We do this by setting up a Dirac equation in a rotating frame of reference and using its solutions to build wave packets whose angular momentum properties can be analyzed. Throughout we retain constants in our equations, but diagrams are drawn in units where \( \hbar = c = m = 1 \).

This paper is set out as follows. First we discuss the derivation of the Dirac equation for an observer in a rotating frame of reference. Then we find the full solutions of it for free particles, which introduces a time-dependent phase into the wave functions. Next we solve the Dirac equation in certain limiting cases to provide greater insight into the full solutions. The next step is to create localized wave packets from these solutions and analyze their properties as a function of the angular momentum of the observer. Finally we draw conclusions about the nature of spin and orbital angular momentum in a relativistic context.

II. DIRAC EQUATION

The Dirac equation in a general noninertial frame in Cartesian and cylindrical coordinates has been derived by Hehl and Ni [13] and Strange and Ryder [14] using standard methods [15–18]. Here we restrict ourselves to Cartesian coordinates and a rotating frame with no linear acceleration. The Dirac equation in an observer’s noninertial frame is then [13]

\[
i\hbar \frac{\partial}{\partial t} \psi(r,t) = (\alpha \cdot \mathbf{p} + \beta \hbar c^2) \psi(r,t) - \omega \cdot \left( \mathbf{r} \times \mathbf{p} + \frac{\hbar}{2} \right) \psi(r,t),
\]

(1)

*Corresponding author: P.Strange@kent.ac.uk
where \( \omega \) is the vector angular frequency of the reference frame (the observer) relative to an inertial frame and the other symbols take on their usual meanings [19]. Equation (1) is exact when we start from a rotating Minkowski metric. It is interesting to note that the coupling to the angular frequency of the observer through the spin operator and through the orbital angular momentum operator individually contributes to the full solution. This tells us there is no frame in which the current density is volume are

\[
\frac{i}{\hbar} \frac{\partial}{\partial t} \psi(r,t) = (\mathbf{c} \cdot \mathbf{p} + \beta m c^2) \psi(r,t) - \omega (\hat{L}_z + \hat{S}_z) \psi(r,t).
\]

(3)

This arrangement has been chosen because classically the spin and orbital angular momentum become indistinguishable when they are considered around the same axis. Given the contrasting nature of the corresponding operators it seems unlikely that their effect on the eigenfunction will be indistinguishable. The probability and current densities associated with this equation are respectively

\[
\rho(r,t) = \psi^\dagger(r,t) \psi(r,t),
\]

\[
f(r,t) = \psi^\dagger(r,t) (\mathbf{c} \cdot \mathbf{a} + \omega \times \mathbf{r}) \psi(r,t).
\]

(4)

We find restricted solutions of Eq. (3). If we consider motion only in the \( xy \) plane the Dirac equation partially decouples. \( \psi(r,t) \) is a four-component quantity in general, but in this case the first and fourth components become decoupled from the second and third. Therefore we can solve for the cases where either the second and third component of \( \psi(r,t) \) or the first and fourth component are zero. This simplifies the mathematics, but does not affect the physics we wish to describe.

III. SOLUTIONS

Equation (3) is derived from the most fundamental form of the Dirac equation [13] and the space-time metric of our rotating frame. Our next task is to find its free particle solutions. First we find its full solutions. The angular frequency of the observer couples to the particle through the spin and the orbital angular momentum separately. This equation cannot be changed in any realistic way. However to observe how spin and orbital angular momentum terms contribute separately to the full solution we have also solved Eq. (3) with the \( \hat{L}_z \) and \( \hat{S}_z \) operators set equal to zero in turn. These latter solutions have no physical meaning in themselves. However they do allow us to see how coupling of the angular frequency of the observer through the spin operator and through the orbital angular momentum operator individually contribute to the full solution. Looked at in reverse, this enables us to gain insight into the role of the orbital angular momentum operators, and particularly the nonrelativistic spin operator, and hence gain insight into what this operator actually tells us.

A. Full solution

First we look at the full solutions with the coupling to the angular frequency of the observer through both \( \hat{L}_z \) and \( \hat{S}_z \) included. The positive energy solutions normalized to unit volume are

\[
\psi_1(r,t) = \left( \frac{W + mc^2}{2W} \right)^{1/2} \begin{pmatrix} \exp(i\omega t/2) \\ 0 \\ \frac{\hbar(k_1 + i k_2)}{W + mc^2} \exp(-i\omega t/2) \\ 0 \end{pmatrix} \times e^{i(\omega - W t/\hbar)},
\]

(5)

\[
\psi_2(r,t) = \left( \frac{W + mc^2}{2W} \right)^{1/2} \begin{pmatrix} 0 \\ \frac{\hbar(k_1 - i k_2)}{W + mc^2} \exp(-i\omega t/2) \\ \exp(i\omega t/2) \\ 0 \end{pmatrix} \times e^{i(\omega - W t/\hbar)},
\]

(6)

where \( k_1 \) and \( k_2 \) are arbitrary wave vectors,

\[
W = \sqrt{m^2 c^4 + \hbar^2 c^2 (k_1^2 + k_2^2)}
\]

(7)

is related, but not equal, to the total energy, and \( u \) is defined as

\[
u = x(k_1 \cos \omega t + k_2 \sin \omega t) + y(k_2 \cos \omega t - k_1 \sin \omega t).
\]

(8)

The \( \omega \) dependence here interesting. It is the observer who is in a noninertial frame rotating with angular frequency \( \omega \). Therefore he sees the particle, which has constant velocity in an inertial frame, as rotating. This is accounted for by the \( u \) in the exponent. However there is an additional phase in the matrix part of the wave function which differs for each component and which is dependent on the angular frequency of the observer. This is a surprising feature of these solutions. In an inertial frame (\( \omega = 0 \)) both components of the wave function have a well-defined and constant phase relation, but if we move to a rotating frame there is an additional phase which varies with time. This phase is \( \exp(i\omega t/2) \) in the spin-up channels of the eigenfunction and \( \exp(-i\omega t/2) \) in the spin-down channels, although it is time dependent and depends on \( \omega \), which is unrelated to the particle spin. As we show below this phase arises from the orbital angular momentum operator in the Hamiltonian. In the probability density these phases cancel. However, the probability current density includes an off-diagonal matrix operator which connects different components of the wave function and in this case the time dependence does not cancel. This tells us there is no frame in which the current density is stationary. It is also noteworthy that \( \omega \) does not appear outside the exponents, even in the quantity \( W \), so the probability
density $\rho(r,t)$ is independent of $\omega$, although again, this is not true for the current density. We note, for future reference, that $W$ takes on the same form as the total energy of a free particle in an inertial frame of reference. Similar expressions to (5) and (6) can easily be found for the negative energy solutions.

It is well known that if the inertial Dirac equation is solved in an electromagnetic field and either the nonrelativistic limit is taken or a Foldy-Wouthuysen transformation is performed the magnetic moment (spin) of the electron drops out of the calculation. The spin can also be deduced from Eq. (3). If we let $\hat{S}_c = a\hbar\sigma_z$ and minimize the sum of the $W$’s for a spin-up and a spin-down particle with respect to $a$ we find $a = 1/2$.

**B. Solution in the limit of zero spin**

If we set $\hat{S}_c = 0$ in Eq. (3) we no longer have a derived equation. Our reason for setting $\hat{S}_c = 0$ is simply to look at the contribution of the orbital angular momentum to the full solution. The probability density is still as given by Eq. (4).

**Our positive energy wave functions are**

$$\psi_1(r,t) = \left(\frac{W_s + mc^2 + \hbar\omega/2}{2W_L}\right)^{1/2} \begin{pmatrix} 1 \\ 0 \\ -\frac{\hbar(c_k + i\kappa)}{W_L + mc^2 + \hbar\omega/2} \exp(-i\omega t/\hbar) \\ 0 \end{pmatrix} e^{i(u - \omega t)/\hbar},$$

$$\psi_2(r,t) = \left(\frac{W_s + mc^2 - \hbar\omega/2}{2W_L}\right)^{1/2} \begin{pmatrix} 0 \\ e^{-i\omega t/\hbar} \\ \frac{\hbar(c_k - i\kappa)}{W_L + mc^2 - \hbar\omega/2} \exp(i\omega t/\hbar) \\ 0 \end{pmatrix} e^{i(u - \omega t)/\hbar},$$

where $W_L$ is given by

$$W_L = \sqrt{mc^4 + \hbar^2 c^2(k_1^2 + k_2^2) \pm \hbar mc^2 + \hbar^2 \omega^2/4}.$$

The only appreciable difference between this case and the full solution is the occurrence of $\omega$ in the prefactors and the definition of $W_L$. We see here that the $\exp(\pm i\omega t/2)$ that appeared in the full solutions also appears here, so must arise from the coupling of the angular frequency of the observer to the orbital angular momentum. In the expression for $W_L$ the $+(-)$ refer to $\psi_1(\psi_2)$ respectively. This means that $W_L$ depends on whether $\omega$ is parallel or antiparallel to the spin direction. The presence of the orbital angular momentum operator in the Dirac equation means that it is not appropriate to separate the time and spatial parts of the eigenfunctions and results in the particular form of $u$ given in Eq. (8). In turn, this means $W_L$ cannot be identified with the total energy. As in the full solutions the time dependence cancels in the probability density, but not in the current density.

**C. Solution in the limit of zero orbital angular momentum**

Again, if we set $\hat{L}_c = 0$ we do not have a derived equation, but setting $\hat{L}_c = 0$ allows us to look at the contribution of the coupling of $\omega$ through the spin operator to the full solution. The probability density remains as given by Eq. (4) but the term in $\omega \times r$ disappears in the current density. Our positive energy eigenfunctions in this case are

$$\psi_1(r,t) = \left(\frac{W_s + mc^2 - \hbar\omega/2}{2W_s}\right)^{1/2} \begin{pmatrix} 1 \\ 0 \\ \frac{\hbar(c_k + i\kappa)}{W_s + mc^2 - \hbar\omega/2} \exp(i(k_x + \kappa_2 y - \omega t/\hbar)) \\ 0 \end{pmatrix},$$

$$\psi_2(r,t) = \left(\frac{W_s + mc^2 + \hbar\omega/2}{2W_s}\right)^{1/2} \begin{pmatrix} 0 \\ 1 \\ \frac{\hbar(c_k - i\kappa)}{W_s + mc^2 + \hbar\omega/2} \exp(i(k_x + \kappa_2 y - \omega t/\hbar)) \\ 0 \end{pmatrix}$$

with eigenvalue $W_s$ given by

$$W_s = \sqrt{mc^4 + \hbar^2 c^2(k_1^2 + k_2^2) \mp \hbar mc^2 + \hbar^2 \omega^2/4}.$$
shown in Fig. 1. In the upper left we show the probability density as a function of position. It is circularly symmetric, clearly has a peak at the origin, and is identical for the spin-up and spin-down cases. In Figs. 1(b) and 1(d) we display the current density where the spin-up and spin-down nature of the two wave functions is evident in its direction of rotation. Finally in Fig. 1(c) we show the current density along the x axis for the case of Fig. 1(b). This figure is reversed for the opposite spin case. The origin of the opposite senses of rotation in these figures is the ±ik2 in the smaller component of the eigenfunctions coupled to the signs of the nonzero elements of \( \alpha \), in Eq. (4) and the fact that we have a wave packet that is symmetric in \( k_1 \) and \( k_2 \). This gives the lower component of the eigenfunctions a different phase from the upper component and interference between the components when put together as prescribed by Eq. (4) yields the rotational behavior shown in Fig. 1. These figures look similar regardless of whether we choose Eqs. (5) and (6) or (9) and (10) or (12) and (13) to create the wave packet.

It is instructive to look at both the probability density and the current density as a function of \( \omega \). The probability density is the sum of two terms. First there is a curve that reflects \( a(k_1,k_2) \) arising from the large component of the eigenfunction. Second there is a function that has a zero at the origin, and two peaks either side close to where the large component has the highest gradient, which arises from the small component. These are shown in Fig. 2. If \( \omega \) is small as in Fig. 1 the probability density has a single peak at the origin. However for large \( \omega \) the small component can dominate and then there is a circular maximum reflecting the spreading of the wave packet. If we set \( \hat{S}_z = 0, \hat{L}_z \neq 0 \) in the Dirac equation (3) and find the solutions, the transitions take place in essentially the same frequency range and the picture is very similar, so it is not shown in Fig. 3. Very slight differences between the two cases are due to the frequency dependence of the normalization in the \( \hat{S}_z = 0 \) case.

FIG. 1. (a) The probability density and (b) the current density for the wave function (15) with \( \eta_1 = 1, \eta_2 = 0, \omega = 0 \) and the width of the Gaussian envelope \( \sigma = 0.4 \), evaluated at time \( t = 0.4 \). (c) The current density of (b) along the x axis. (d) The same as (b) but for \( \eta_1 = 0 \) and \( \eta_2 = 1 \). All quantities are displayed in relativistic units (\( m = \hbar = c = 1 \)).

FIG. 2. The components of the probability density on the line \( y = 0 \). The wave packet is defined by Eq. (15) with a Gaussian profile with \( \sigma = 0.4, \omega = 0.2 \) and \( \eta_1 = 1, \eta_2 = 0 \) and evaluated at \( t = 0 \). The full blue line is the contribution from the large component of the wave function and the dotted green line is the contribution from the small component (multiplied by 20 for clarity). All quantities are in relativistic units (\( m = \hbar = c = 1 \)).
This leads us to conclude that change in the sense of rotation of the wave packet is due to the coupling of the angular frequency of the observer to the \( L_z \) operator.

Figure 3(b) shows the same quantity when we couple the particle to the rotation through \( \hat{S}_z \) only. Remarkably, in this case neither \( j_y (r, t) \) nor \( j_z (r, t) \) are ever equal to zero as a function of angular frequency of the observer and so do not change sign; the direction of the current density is independent of \( \omega \). The curves tend asymptotically to zero as \( \omega \to \pm \infty \). Although we apparently have rotational motion in Fig. 1, there is no angular frequency of the observer at which the wave packet appears to change its sense of rotation when the rotation of the observer couples to the wave packet only through the spin operator. The results shown in Fig. 3(b) are due to a small but key detail in the eigenfunctions of the spin-only equation. The coefficients of the exponential in Eqs. (5) and (6) are independent of \( \omega \). This is not the case for Eqs. (12) and (13) where both the large and small components of the wave function depend weakly on \( \omega \), through the normalization, and the denominator in the matrix part of Eqs. (12) and (13). The quantity \( W_t + mc^2 - \hbar \omega / 2 \) is never nonpositive, but becomes small for large \( \omega \). This means that \( \omega \) can be tuned to maximize the small component of the eigenfunction when \( L_z = 0 \). For example, in Eq. (12) when \( \omega \) is large and negative the probability density reflects the Gaussian contribution (full blue curve in Fig. 2). As \( \omega \) passes through zero and becomes positive the small component of the wave function begins to dominate and the probability density becomes two-peaked (green dotted curve in Fig. 2). This occurs because the \( -\hbar \omega / 2 \) in the denominator of the small component makes that denominator small and the contribution of that component to the probability density becomes large. The same happens in Eq. (13) at frequencies that are large and negative. If we set \( \hat{S}_z = 0, \hat{L}_z \neq 0 \) we can see from Eqs. (9) and (10) that a similar thing occurs with opposite signs. In the eigenfunction of Eq. (9) it is when \( \omega \) becomes large and negative that there is a maximum in the small component of the eigenfunction. Surprisingly, and despite the fact that the spin and the orbital angular momentum operators are very different, when both \( \hat{S}_z \) and \( \hat{L}_z \) are included in the calculation, the \( \omega \) dependence in the prefactors cancels and the small component of the wave function remains small for all values of \( \omega \). This is also the origin of the anisotropy in the right-hand picture in Fig. 3. To the left of this peak in this diagram the large component of the wave function tends to dominate much of the wave packet, while to the right of the peak the small component is more important.

We have calculated \( \langle S_z \rangle = \langle \hbar \sigma_z / 2 \rangle \) as a function of \( \omega \) for identical wave packets composed of solutions of Eqs. (5), (9), and (12) and display the results in Fig. 4. The angular frequencies shown on this figure are huge and most are not experimentally accessible. Nevertheless we show it to illustrate the mathematics. For the full solution \( \langle S_z \rangle \) is constant. This is shown as the full red line in Fig. 4. Mathematically this is because the exponentials cancel when we calculate the expectation value and the angular frequency does not appear anywhere else in the eigenfunctions (5). The rotation of the observer causes the apparent orbital angular momentum of the particle to change, but not its spin. This is as expected. The short dashed blue line in Fig. 4 is the value of \( \langle S_z \rangle \) when we couple the angular frequency of the observer to the particle through the spin operator only. Clearly this gives a value close to \( \langle S_z \rangle = 1/2 \) for negative angular frequencies but falls off rapidly for positive values of \( \omega \). Finally the long dashed green line in Fig. 4 is \( \langle S_z \rangle \) when we couple the angular frequency of the observer to the particle through the orbital angular momentum operator only. In this case the results are good for positive frequencies, but fall off rapidly for negative frequencies. Figure 4 is unexpectedly symmetric about \( \omega = 0 \). In fact we can see from the eigenfunctions that Eq. (9) with negative frequency and Eq. (12) with positive frequency are identical at \( t = 0 \). This symmetry remains at later times because the time only appears in exponential which cancels.

FIG. 3. The x and y components of the current density at a particular point in space as a function of angular frequency \( \omega \). All quantities are in relativistic units \( \hbar = m = c = 1 \). The wave packet is defined by Eq. (15) with a Gaussian profile with \( \sigma = 0.4 \) and \( \eta_1, \eta_2 = 0 \) and evaluated at \( t = 0 \). Left: when the observer interacts with the wave packet through both the spin and orbital angular momentum operators so \( \psi_1 \) is given by Eq. (5). Right: when the observer interacts with the wave packet only through the spin operator so \( \psi_1 \) is given by Eq. (12).
when we evaluate the expectation value of diagonal operators. These latter results have no meaning by themselves, but they do show that there is a remarkable cancellation between the effects of the spin and orbital angular momentum terms in Eq. (3) to give \( \langle S_z \rangle \) independent of the angular frequency of the observer. In the case where the coupling is through the spin operator, \( \langle S_z \rangle \) changes sign as a function of \( \omega \), but the angular rotation of the current density does not. This is not consistent with Figs. 1(b) and 1(d) where \( \langle S_z \rangle \) changes sign and spin-up and spin-down wave packets are represented by the current rotating in opposite directions. We attribute this discrepancy to \( \hbar \sigma_z/2 \) being a good operator to describe spin at low angular frequencies, but at high angular frequencies, when relativistic effects become important, it is no longer the appropriate operator. This supports the well-known fact that \( S_z = \hbar \sigma_z/2 \) needs to be modified because it does not commute with the Dirac free particle Hamiltonian and so does not represent a conserved quantity; a new spin operator is needed.

V. CONCLUSIONS

The Dirac equation for an observer in a rotating frame of reference (1) contains terms coupling the rotational motion of the observer to the system under observation through the nonrelativistic orbital angular momentum and spin operators. We have solved this equation for free particles exactly and used the solutions to create localized wave packets. Reassuringly the magnitude of the particle spin emerges correctly from these equations even without an electromagnetic field being present. We have demonstrated unexpected behavior of relativistic wave packets. In particular we have shown that the coupling through the orbital angular momentum operator leads to the wave functions having a time-dependent phase which differs between the components of the wave function. It is the orbital angular momentum operator which directly couples the rotation of the observer to the particle. The fact that the apparent direction of the rotation of the current density can be reversed by adjusting the observer’s angular frequency relative to the wave packet through this operator illustrates and proves this point. On top of this classical rotation of the wave packet, the orbital angular momentum operator also changes the weight of the spin-up and spin-down character in the wave packets causing a secondary change in apparent magnitude of the rotation.

The coupling of the rotational motion of the observer to the wave packet through the spin operator does not mechanically change the direction of rotation directly. It only changes the relative amounts of spin-up and spin-down character in the wave packet, thus changing the magnitude of the rotation indirectly. Remarkably it does this at exactly the right level to cancel the changes in the weight of the spin-up and spin-down character in the wave packets caused by the orbital angular momentum operator as shown by our calculation of \( \langle S_z \rangle \). It is only this cancellation that keeps the small component of the wave function actually small at all angular frequencies. It is also this cancellation that means the effect of the combined spin and orbital angular momentum operators in the Dirac equation (3) is to produce a simple classical rotation of the wave packet. Neither the spin nor the orbital angular momentum operators yield a completely classical rotation themselves, but together it seems that they do.

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