SPIN-DEPENDENT BOHM TRAJECTORIES
FOR PAULI AND DIRAC EIGENSTATES OF HYDROGEN

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The de Broglie-Bohm causal theory of quantum mechanics is applied to the hydrogen atom in the fully spin-dependent and relativistic framework of the Dirac equation, and in the nonrelativistic but spin-dependent framework of the Pauli equation. Eigenstates are chosen which are simultaneous eigenstates of the energy H, total angular momentum M, and z component of the total angular momentum M_z. We find the trajectories of the electron, and show that in these eigenstates, motion is circular about the z-axis, with constant angular velocity. We compute the rates of revolution for the ground ($n = 1$) state and the $n = 2$ states, and show that there is agreement in the relevant cases between the Dirac and Pauli results, and with earlier results on the Schrödinger equation.

Key words: de Broglie-Bohm theory, Bohm trajectories, causal interpretation of quantum mechanics, relativistic quantum theory.

1. INTRODUCTION

In Bohm's original causal interpretation of quantum mechanics [2], the motion of a quantum particle is determined by its Schrödinger wave function ψ, which acts as a kind of guidance wave [6]. If the wave function is written as

$$\psi(\mathbf{x}, t) = R(\mathbf{x}, t)e^{iS(\mathbf{x},t)/\hbar}, \tag{1}$$

where R and S are real-valued, then the trajectory of the particle is determined by the guidance relation

$$\mathbf{p} = \nabla S. \tag{2}$$

The momentum is related to the well-known Schrödinger current $\mathbf{j}$ as follows,

$$\mathbf{p} = \frac{m}{\rho}\mathbf{j}, \tag{3}$$

where $\rho = \psi^\dagger\psi = R^2$. Comprehensive discussions of the de Broglie-Bohm causal interpretation can be found in [3] and [10].

It is quite natural to examine the hydrogen atom, one of the simplest quantum systems, in terms of the de Broglie-Bohm theory. Indeed, as originally discussed in [2], the Schrödinger guidance relation (2) predicts that $\mathbf{p} = \mathbf{0}$ for all real eigenstates, including the ground and all higher s hydrogenic states. However, as Holland [11] pointed out, Eq. (2) is valid only for spinless particles. For particles with spin, the condition of Lorentz covariance on the law of motion implies that the momentum of a particle with spin $\mathbf{s}$ must be given by

$$\mathbf{p} = \nabla S + \nabla \log \rho \times \mathbf{s}, \tag{4}$$

where $\rho = \psi^\dagger\psi$ [9, 11]. Only in this way can the theory be embedded in a relativistic formulation. Indeed, in papers [7, 8, 9], it was shown that in order for it to be consistent with Dirac theory, the Schrödinger equation must be regarded as describing an electron in a definite eigenstate of spin. In these papers, the current vector associated with (4),

$$\mathbf{j} = \frac{1}{m}\rho\nabla S + \frac{1}{m}\nabla\rho \times \mathbf{s}, \tag{5}$$

was referred to as the *Pauli current*, the nonrelativistic limit of the *Dirac current*.

The guidance law (4) no longer implies that $\mathbf{p} = \mathbf{0}$ for real eigenstates so it is natural to ask how it applies to the hydrogen atom. In [5], we showed that for an electron in a spin eigenstate with $s_z = \pm\frac{1}{2}$, the spin-dependent term in (4) will be responsible for a motion in a plane perpendicular to the z-axis and along a contour of constant ρ value. For the case of an electron in a Schrödinger energy/angular momentum eigenstate, ψ_{nlm}, this implies circular motion about the z-axis.

In this paper, we examine de Broglie-Bohm trajectories for an electron in a hydrogen atom as described by the Pauli and Dirac equations using appropriate (spin-dependent) currents. The electron is assumed to be in a Pauli or Dirac eigenstate of energy and total angular

momentum. Note that, in general, this does not imply that the electron is in a spin eigenstate of known s_z value. We also show that under appropriate nonrelativistic limits, the angular rotation rates for Dirac trajectories become those of Pauli trajectories. In the cases that the electron is in a spin eigenstate (e.g., $1s$, $2s$, $2p_0$), the Pauli rotation rates agree with the Schrödinger trajectories obtained in [5]. The result is a coherent application of de Broglie-Bohm theory to relativistic and nonrelativistic hydrogen atom eigenstates.

For both the Dirac and Pauli cases, the Schrödinger guidance formula in (4) can be generalized using the relationship (3) where $\mathbf{j}$ is the appropriate (Dirac/Pauli) current and $\rho = \psi^\dagger \psi$. First, consider the Dirac equation,

$$i\hbar\frac{\partial}{\partial t}\psi = (-e\phi + \beta E_o + \boldsymbol{\alpha} \cdot (c\mathbf{p} + e\mathbf{A}))\psi. \tag{6}$$

Here, $\psi = (\psi_1, \psi_2, \psi_3, \psi_4)$ is a four-component wave function, ϕ and $\mathbf{A}$ are the scalar and vector potentials, E_0 and $\mathbf{p}$ are the rest mass energy and momentum operators, e is the electric charge, and $\boldsymbol{\alpha}$ and β are the Dirac operators. In this study, $\mathbf{A} = 0$ and the current is given by

$$\mathbf{j} = c\psi^\dagger\boldsymbol{\alpha}\psi = (j_x, j_y, j_z), \tag{7}$$

where the $\boldsymbol{\alpha}$ are the 4×4 Dirac matrices,

$$\boldsymbol{\alpha} = \begin{pmatrix} 0 & \sigma \\ \sigma & 0 \end{pmatrix}, \tag{8}$$

and the $\boldsymbol{\sigma}$ are the 2×2 Pauli matrices.

If the particle is in a potential such that $e\phi \ll mc^2$, then there exist stationary states for which the average velocity $\bar{v}$ is nonrelativistic, and $E \approx E_0 = mc^2$. In this case, the latter two components of the 4-component Dirac state are smaller in magnitude than the first two components by a factor of $\bar{v}/c$. The Dirac equation may then be reduced to the Pauli equation involving the two components ψ_1 and ψ_2:

$$i\hbar\frac{\partial\psi}{\partial t} = \frac{1}{2m}(-i\hbar\nabla + e\mathbf{A})^2\psi + \frac{e\hbar}{2m}\boldsymbol{\sigma} \cdot \mathbf{B}\psi - eV\psi. \tag{9}$$

Here $\psi = (\psi_1, \psi_2)$ is a two-component Pauli spinor wave function. Once again, we assume that $\mathbf{A} = 0$ so that the associated Pauli current is given by [3]

$$\mathbf{j} = \mathbf{j}_A + \mathbf{j}_B = \frac{\hbar}{2mi}(\psi^\dagger\nabla\psi - \psi\nabla\psi^\dagger) + \frac{\hbar}{2m}\nabla \times (\psi^\dagger\sigma\psi). \tag{10}$$

Note that if one assumes that the system is in an eigenstate of the spin operator, then (10) and (3) together reduce to (4).

In the case of the Schrödinger equation for hydrogen, it is usually assumed that spin interactions are negligible so that the wave function can be written as a product of spatial- and spin-dependent terms, i.e.,

$$\psi = \psi(\mathbf{r}, t)\chi_s. \tag{11}$$

As is well known, the spatial hydrogenic energy Schrödinger eigenfunctions,

$$\psi_{n,\ell,m}(r, \theta, \phi) = R_{n,\ell}(r)Y_{lm}(\theta, \phi), \tag{12}$$

solutions to the (spinless) time-independent Schrödinger equation, are also simultaneous eigenstates of the orbital angular momentum operator L^2, with eigenvalues $\hbar^2\ell(\ell + 1)$, and the operator L_z, with eigenvalues $\hbar m$.

In the Pauli equation, where spin-orbit interactions are excluded, the orbital angular momentum operator L^2 commutes with the hamiltonian. This is not the case for the Dirac equation. For both the Pauli and Dirac equations, however, each component of M, the total angular momentum operator, commutes with the Hamiltonian H, implying that M^2 commutes with H as well. For this reason, it is conventional to choose eigenstates of H, M^2 and M_z, with eigenvalues E_n, $\hbar^2 j(j + \frac{1}{2})$ and $\hbar m$, respectively.

There is one further subtlety: Although the orbital angular momentum does not commute with the hamiltonian in the Dirac case, it can be shown that ℓ is 'almost' a good quantum number (see [1]). That is to say, eigenstates can be found for which

$$\mathbf{L}^2\psi = \hbar^2\ell(\ell + 1)\psi + \hbar^2 w, \tag{13}$$

where the spinor w is negligible. (Its large components actually vanish.) Hence for both the Dirac and Pauli cases considered in this paper, eigenstates are presented in terms of quantum numbers n, ℓ, j and m for purposes of comparison, even though ℓ is not strictly a good quantum number in the Dirac case.

Finally, in the following discussions, the time-dependent phase factor $e^{-iE_n t/\hbar}$ that accompanies the eigenfunctions in the solution of the time-dependent Pauli and Dirac equations will be ignored since it contributes nothing to the associated currents.

2. PAULI EIGENSTATES

In this section we examine the Pauli current (10) for some hydrogen atom eigenstates. These eigenstates, two-component solutions to the

Pauli equation, are given by [1]

$$
\psi_{n,\ell,j=\ell+\frac{1}{2},m} = \frac{1}{\sqrt{2\ell+1}} R_{n\ell}(r) \begin{pmatrix} \sqrt{\ell+m+\frac{1}{2}} \, Y_{\ell,m-\frac{1}{2}}(\theta,\phi) \\ -\sqrt{\ell-m+\frac{1}{2}} \, Y_{\ell,m+\frac{1}{2}}(\theta,\phi) \end{pmatrix},
$$

$$
\psi_{n,\ell,j=\ell-\frac{1}{2},m} = \frac{1}{\sqrt{2\ell+1}} R_{n\ell}(r) \begin{pmatrix} \sqrt{\ell-m+\frac{1}{2}} \, Y_{\ell,m-\frac{1}{2}}(\theta,\phi) \\ \sqrt{\ell+m+\frac{1}{2}} \, Y_{\ell,m+\frac{1}{2}}(\theta,\phi) \end{pmatrix}. \tag{14}
$$

Here, the $R_{nl}(r)$ are the standard radial wave functions for the hydrogen atom and the $Y_{l,m\pm\frac{1}{2}}(\theta,\phi)$ are the spherical harmonics.[1] We use spherical polar coordinates in which r is the radius, ϕ is the angle measured counterclockwise from the x-axis and θ is the angle measured down from the z-axis.

As mentioned earlier, the wave functions given in (14) are eigenfunctions of L^2 (the orbital angular momentum) with eigenvalue $\hbar^2\ell(\ell+1)$, M^2 (the total angular momentum) with eigenvalue $\hbar^2 j(j+1)$ and M_z with eigenvalue $m\hbar$. In general, however, they are *not* eigenstates of s_z, the projection of spin along the z-axis.

The eigenfunctions can be classified as follows:

- For each n value, ℓ can assume the values $\ell = 0, 1, ..., n-1$.

- For each ℓ value, m can assume the values $m = -\ell + 1/2, -\ell + 3/2, ..., \ell - 1/2$.

- For each of the above there are two possibilities, $j = \ell + 1/2$ and $j = \ell - 1/2$.

This accounts for all eigenfunctions listed in (14).

From (10), the two contributions to the velocity are given by

$$
\mathbf{v}_a = \frac{\mathbf{j}_a}{\rho} = \frac{\hbar}{2m_e i} \frac{(\psi^\dagger \nabla \psi - \psi \nabla \psi^\dagger)}{\psi^\dagger \psi} = \frac{\hbar}{m_e} \frac{\mathrm{Im}(\psi^\dagger \nabla \psi)}{\psi^\dagger \psi} \tag{15}
$$

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[1]We use the following convention for the relevant functions, for consistency with [1]:

$$
Y_{\ell m}(\theta,\phi) = \frac{1}{\sqrt{2\pi}} P_{\ell m}(\cos\theta) e^{im\phi},
$$

$$
P_{\ell m}(x) = \sqrt{\frac{2\ell+1}{2} \frac{(\ell-m)!}{(\ell+m)!}} \frac{1}{2^\ell \ell!} (1-x^2)^{m/2} \frac{d^{\ell+m}}{dx^{(\ell+m)}} (x^2-1)^\ell, \quad m \geq 0,
$$

$$
P_{\ell,-m}(x) = (-1)^m P_{\ell m}(x), \quad m < 0.
$$

and

$$\mathbf{v}_b = \frac{\mathbf{j}_b}{\rho} = \frac{\hbar}{2m_e}\frac{\nabla \times \mathbf{s}}{\psi^\dagger\psi}, \tag{16}$$

where

$$\mathbf{s} = \psi^\dagger \sigma \psi \tag{17}$$

is the 'spin vector' and m_e is the mass of the electron. In order to determine trajectories for the above hydrogen eigenstates we must compute the velocities $\mathbf{v}_a$ and $\mathbf{v}_b$ for the wave functions given in (14).

We first examine the velocity $\mathbf{v}_a$ arising from the Schrödinger current $\mathbf{j}_a$. Writing

$$\psi = \frac{1}{\sqrt{2\ell+1}}R_{n\ell}(r)\begin{pmatrix} v_1(\theta,\phi) \\ v_2(\theta,\phi) \end{pmatrix}, \tag{18}$$

the term $\mathrm{Im}\{\psi^\dagger\nabla\psi\}$ can be shown to be

$$\mathrm{Im}\{\psi^\dagger\nabla\psi\} = \frac{1}{2\ell+1}\mathrm{Im}\Big\{ R_{n\ell}R'_{n\ell}(|v_1|^2+|v_2|^2)\hat{e}_r+\frac{1}{r}R_{n\ell}^2(v_1^*\frac{\partial v_1}{\partial\theta}+v_2^*\frac{\partial v_2}{\partial\theta})\hat{e}_\theta$$
$$+\frac{1}{r\sin\theta}R_{n\ell}^2(v_1^*\frac{\partial v_1}{\partial\phi}+v_2^*\frac{\partial v_2}{\partial\phi})\hat{e}_\phi\Big\}. \tag{19}$$

In the above, the only nonzero term comes from the $\hat{e}_\phi$ component:

$$v_k^*\frac{\partial v_k}{\partial\theta} = i(m\pm\frac{1}{2})|v_k|^2, \qquad k=1,2, \tag{20}$$

so that (15) yields

$$\mathbf{v}_a = \frac{\hbar}{m_e r\sin\theta}\Big(m+\frac{1}{2}\big(\frac{|v_2|^2-|v_1|^2}{|v_1|^2+|v_2|^2}\big)\Big)\hat{e}_\phi. \tag{21}$$

It remains to compute $\mathbf{j}_b$ and the corresponding velocity $\mathbf{v}_b$, with reference to (16). To do this, we first find the three components of the spin vector $\mathbf{s} = \psi^\dagger\sigma\psi$:

$$\psi^\dagger\sigma\psi = \frac{1}{2\ell+1}R_{n\ell}(r)^2\Big(2\mathrm{Re}\{v_1^*v_2\}, 2\mathrm{Im}\{v_1^*v_2\}, |v_1|^2-|v_2|^2\Big). \tag{22}$$

From the form of the wave functions (14),

$$2\mathrm{Re}(v_1^*v_2) = 2c_1c_2N_1N_2P_\ell^{m-\frac{1}{2}}(\theta)P_\ell^{m+\frac{1}{2}}(\theta)\cos\phi \tag{23}$$

and

$$2\text{Im}(v_1^* v_2) = 2c_1 c_2 N_1 N_2 P_\ell^{m-\frac{1}{2}}(\theta) P_\ell^{m+\frac{1}{2}}(\theta) \sin\phi, \tag{24}$$

where the c_i are given in (14) and the N_i are the normalization constants of the relevant spherical harmonics. For simplicity of notation, define

$$a = c_1 N_1 P_\ell^{m-\frac{1}{2}}, \quad b = c_2 N_2 P_\ell^{m+\frac{1}{2}}. \tag{25}$$

If we write

$$\psi^\dagger \sigma \psi = \frac{1}{2\ell + 1} R_{n\ell}^2(r) \mathbf{w}, \tag{26}$$

then the vector $\mathbf{w}$ can be expressed in Cartesian form as

$$(w_x, w_y, w_z) = (2ab\cos\phi, 2ab\sin\phi, a^2 - b^2). \tag{27}$$

We may also express $\mathbf{w}$ in spherical polar form, i.e.,

$$\begin{aligned}
w_x &= r_s \sin\theta_s \cos\phi_s, \\
w_y &= r_s \sin\theta_s \sin\phi_s, \\
w_z &= r_s \cos\theta_s,
\end{aligned} \tag{28}$$

where the orientation of the spin vector $\mathbf{s} = \psi^\dagger \sigma \psi$ is given by the angles θ_s and ϕ_s. (See also [1], p. 62-63 for a brief discussion of the spin vector.) A comparison of (28) with (27) suggests that we might let $r_s = a^2 + b^2$, $\phi_s = \phi$ and then compute θ_s in terms of θ using the relations

$$\cos\theta_s = \frac{a^2 - b^2}{a^2 + b^2}, \qquad \sin\theta_s = \frac{2ab}{a^2 + b^2}. \tag{29}$$

However, this is consistent with the definition of spherical coordinates only if $2ab \geq 0$ since θ_s is restricted to the interval $[0, \pi]$. When this condition is not met, i.e., $2ab < 0$, then the polar coordinates for $\mathbf{w}$ are given by $r_s = a^2 + b^2$, $\phi_s = \phi + \pi$ and

$$\cos\theta_s = \frac{a^2 - b^2}{a^2 + b^2}, \qquad \sin\theta_s = \frac{|2ab|}{a^2 + b^2} = -\frac{2ab}{a^2 + b^2}. \tag{30}$$

In either of the above cases, the spin vector $\mathbf{s}$ lies in a plane defined by the position vector $\mathbf{r}$ and the z axis, which is in agreement with [1]. After some manipulation, we find that

$$\mathbf{s} = s_r \hat{e}_r + s_\theta \hat{e}_\theta, \tag{31}$$

where

$$
\begin{aligned}
s_r &= s\cos\theta(\frac{a^2 - b^2}{a^2 + b^2}) + s\sin\theta\left(\frac{2ab}{a^2 + b^2}\right), \\
s_\theta &= -s\sin\theta(\frac{a^2 - b^2}{a^2 + b^2}) + s\cos\theta\left(\frac{2ab}{a^2 + b^2}\right).
\end{aligned}
\tag{32}
$$

(Here $\hat{e}_r$, $\hat{e}_\theta$ and $\hat{e}_\phi$ are the spherical polar unit vectors at the position of the electron.) Evolution of the position coordinates as the particle follows the trajectory implies that the spin vector precesses about the z-axis. This was originally described by Holland [10].

From the above result we find that

$$
\mathbf{v}_b = \frac{\hbar}{2m_e}\frac{\nabla \times \mathbf{s}}{\psi^\dagger\psi} = \frac{\hbar}{2mrs}\left(s_\theta + r\frac{\partial s_\theta}{\partial r} - \frac{\partial s_r}{\partial\theta}\right)\hat{e}_\phi.
\tag{33}
$$

In other words, as was the case for $\mathbf{v}_a$ in (21), the contribution to the velocity from $\mathbf{v}_b$ is again only in the $\hat{e}_\phi$ direction. Therefore, for all eigenstates of the form in (14), the motion of the electron is in the $\hat{e}_\phi$ direction, i.e. rotational motion about the z axis. This is in qualitative agreement with the Schrödinger results.

The total speed in the $\hat{e}_\phi$ direction is given by $v = v_a + v_b$, i.e.,

$$
v = \frac{\hbar}{m_e r\sin\theta}\left(m + \frac{1}{2}(\frac{|v_2|^2 - |v_1|^2}{|v_1|^2 + |v_2|^2})\right) + \frac{\hbar}{2mrs}\left(s_\theta + r\frac{\partial s_\theta}{\partial r} - \frac{\partial s_r}{\partial\theta}\right).
\tag{34}
$$

In what follows it will be useful to understand the relationship between the velocities for positive and negative (corresponding) values of m. Recall that for $j = \ell + \frac{1}{2}$,

$$
\psi_{n,\ell,j=\ell+\frac{1}{2},m} = \frac{1}{\sqrt{2\ell + 1}}R_{n\ell}(r)\left(
\begin{array}{c}
\sqrt{\ell+m+\frac{1}{2}}\ Y_{\ell,m-\frac{1}{2}}(\theta,\phi) \\
-\sqrt{\ell-m+\frac{1}{2}}\ Y_{\ell,m+\frac{1}{2}}(\theta,\phi)
\end{array}
\right)
\tag{35}
$$

and

$$
Y_{\ell m} = \frac{1}{\sqrt{2\pi}}P_{\ell m}e^{im\phi}, \quad P_{\ell,-m}(x) = (-1)^m P_{\ell m}(x).
\tag{36}
$$

Also, from the derivation above, the spin vector $\mathbf{s}$ is proportional to

$$
\mathbf{w} = (2\mathrm{Re}\{v_1^* v_2\}, 2\mathrm{Im}\{v_1^* v_2\}, |v_1|^2 - |v_2|^2).
\tag{37}
$$

When m is replaced by $-m$, we have (denoting the new term with a superscript $(-)$ and the old with $(+)$)

$$v_1^{(-)} = \sqrt{\ell-m+\frac{1}{2}}Y_{\ell,-m-\frac{1}{2}} = \sqrt{\ell-m+\frac{1}{2}}\frac{1}{\sqrt{2\pi}}(-1)^{m+\frac{1}{2}}P_{\ell,m+\frac{1}{2}}e^{i(-m-\frac{1}{2})\phi} = v_2^{*(+)}.$$
(38)

Similarly,

$$v_2^{(-)} = -\sqrt{\ell+m+\frac{1}{2}}\frac{1}{\sqrt{2\pi}}P_{\ell,-m+\frac{1}{2}}e^{i(-m+\frac{1}{2})\phi}$$
(39)

$$= -\sqrt{\ell+m+\frac{1}{2}}\frac{1}{\sqrt{2\pi}}(-1)^{m-\frac{1}{2}}P_{\ell,m-\frac{1}{2}}e^{-i(m-\frac{1}{2})\phi} = -v_1^{*(+)}.$$
(40)

Therefore,

$$(|v_1|^2 - |v_2|^2)^{(-)} = -(|v_1|^2 - |v_2|^2)^{(+)}$$
(41)

and, furthermore,

$$(v_1^*v_2)^{(-)} = v_2^{(+)}(-v_1^{*(+)}) = (-v_1^*v_2)^{(+)}.$$
(42)

All three components of $\mathbf{w}$ change sign when m is replaced with $-m$ (the other eigenvalues are left unchanged), so that the spin vector in (26) changes sign. Therefore,

$$\mathbf{v}_a^{(-)} = \frac{\hbar}{m_e r \sin\theta}\left(m + \frac{1}{2}\frac{(|v_2|^2 - |v_1|^2)^{(-)}}{(|v_1|^2 + |v_2|^2)^{(-)}}\right)\hat{e}_\phi = -\mathbf{v}_a^{(+)}$$
(43)

and

$$\mathbf{v}_b^{(-)} = \frac{\hbar}{2m_e}\frac{\nabla \times \mathbf{s}^{(-)}}{\psi^\dagger\psi} = -\mathbf{v}_b^{(+)}.$$
(44)

Thus, both $\mathbf{v}_a$ and $\mathbf{v}_b$ change sign when m changes sign, so that the overall velocity simply changes direction. This simplifies the computation of the rates of revolution. A similar proof holds for the case $j = \ell - \frac{1}{2}$.

Before concluding this section, we mention that in their treatment of the Pauli equation using Euler angles, Bohm and Schiller [4] (p. 80) deduced that the electron in a hydrogen atom eigenstate would execute circular motion about the principal axis with constant angular velocity. However, no angular velocities were computed in the paper. In the next section we compute the angular velocities for the first few Pauli hydrogen eigenstates.

Quantum Number n, ℓ, j, m	Rotation rate $d\phi/dt$
$1, 0, \frac{1}{2}, \pm\frac{1}{2}$	$\pm\frac{\hbar}{m_e ar}$
$2, 0, \frac{1}{2}, \pm\frac{1}{2}$	$\pm\frac{\hbar}{2m_e ar}\left(\frac{1}{1-\frac{r}{2a}}+1\right)$
$2, 1, \frac{3}{2}, \pm\frac{3}{2}$	$\pm\frac{\hbar}{2m_e ar}$
$2, 1, \frac{1}{2}, \pm\frac{1}{2}$	$\pm\frac{\hbar}{m_e r^2}\left(3-\frac{r}{2a}\right)$
$2, 1, \frac{3}{2}, \pm\frac{1}{2}$	$\pm\frac{\hbar}{2m_e ra}\frac{8\cos^2\theta-\sin^2\theta}{4\cos^2\theta+\sin^2\theta}$

Table 1. Angular rates of revolution for Pauli eigenstates

2.1.   Angular Velocities for $n = 1$ and $n = 2$ Pauli Eigenstates

We have computed explicitly the rates of revolution $d\phi/dt$ for the first few Pauli hydrogen eigenstates following the procedure described above. In each case, one computes the velocity $\mathbf{v}_a$, followed by the spin vector $s = \psi^\dagger\psi$, finding s_r and s_θ from (32). Then $\mathbf{v}_b$ is computed to give the total velocity $\mathbf{v}$. Since, for all cases, $\mathbf{v}$ points in the $\hat{e}_\phi$ direction, the angular velocity $d\phi/dt$ is given by

$$\frac{d\phi}{dt} = \frac{v}{r\sin\theta}. \qquad (45)$$

The results of our computations are presented in Table 1.

The first three results presented in Table 1 correspond to wave functions that are also eigenstates of s_z because of the special coupling of spin and orbital angular momentum vectors. As expected, these rates of revolution agree with those computed in [5] for, respectively, the $1s$, $2s$ and $2p_0$ Schrödinger eigenstates. However, the final two states in Table 1 are not spin eigenstates. As such, they have no analogue in the Schrödinger case so that no comparisions of rates can be made.

3. DIRAC EIGENSTATES

We now consider the 4-component Dirac eigenstates for hydrogen. Following [1], they are given as follows: For $j = \ell + \frac{1}{2}$,

$$
\begin{aligned}
\psi_1 &= g(r)\sqrt{\frac{\ell + m + \frac{1}{2}}{2\ell + 1}} Y_{\ell, m - \frac{1}{2}}(\theta, \phi), \\
\psi_2 &= -g(r)\sqrt{\frac{\ell - m + \frac{1}{2}}{2\ell + 1}} Y_{\ell, m + \frac{1}{2}}(\theta, \phi), \\
\psi_3 &= -if(r)\sqrt{\frac{\ell - m + \frac{3}{2}}{2\ell + 3}} Y_{\ell + 1, m - \frac{1}{2}}(\theta, \phi), \\
\psi_4 &= -if(r)\sqrt{\frac{\ell + m + \frac{3}{2}}{2\ell + 3}} Y_{\ell + 1, m + \frac{1}{2}}(\theta, \phi);
\end{aligned}
\tag{46}
$$

and, for $j = \ell - \frac{1}{2}$,

$$
\begin{aligned}
\psi_1 &= g(r)\sqrt{\frac{\ell - m + \frac{1}{2}}{2\ell + 1}} Y_{\ell, m - \frac{1}{2}}(\theta, \phi), \\
\psi_2 &= g(r)\sqrt{\frac{\ell + m + \frac{1}{2}}{2\ell + 1}} Y_{\ell, m + \frac{1}{2}}(\theta, \phi), \\
\psi_3 &= -if(r)\sqrt{\frac{\ell + m - \frac{1}{2}}{2\ell - 1}} Y_{\ell - 1, m - \frac{1}{2}}(\theta, \phi), \\
\psi_4 &= if(r)\sqrt{\frac{\ell - m - \frac{1}{2}}{2\ell - 1}} Y_{\ell - 1, m + \frac{1}{2}}(\theta, \phi).
\end{aligned}
\tag{47}
$$

The $Y_{\ell,m}$ are the usual spherical harmonics and $f(r)$ and $g(r)$ are the normalized radial Dirac eigenfunctions (see [1] p. 69). Recall that even though ℓ is not a good quantum number, the eigenstates are written in terms of ℓ because it is 'almost' a good quantum number, and also because these solutions to the Dirac equation are built from the corresponding Pauli eigenstates. (For a complete discussion, see [1].)

3.1. Trajectories for Generic Dirac Eigenstates

In this section, we show that Bohm trajectories for Dirac hydrogen share common features. First, the components of the Dirac current in

(7) may be expressed in terms of the components of the wave function as follows,

$$\frac{1}{c}j_x = 2\mathrm{Re}\{\psi_1^\dagger\psi_4\} + 2\mathrm{Re}\{\psi_2^\dagger\psi_3\},$$

$$\frac{1}{c}j_y = 2\mathrm{Im}\{\psi_1^\dagger\psi_4\} - 2\mathrm{Im}\{\psi_2^\dagger\psi_3\}, \tag{48}$$

$$\frac{1}{c}j_z = 2\mathrm{Re}\{\psi_1^\dagger\psi_3\} - 2\mathrm{Re}\{\psi_2^\dagger\psi_4\}.$$

We now compute these components using the hydrogenic wave functions given in (46) and (47). Starting with the z component, we find that in the $j = \ell + \frac{1}{2}$ case,

$$\psi_1^\dagger\psi_3 = -if(r)g(r)\sqrt{\frac{\ell + m + \frac{1}{2}}{2\ell + 1}}\sqrt{\frac{\ell - m + \frac{3}{2}}{2\ell + 3}}Y_{\ell,m-\frac{1}{2}}(\theta,\phi)^*Y_{\ell+1,m-\frac{1}{2}}(\theta,\phi) \tag{49}$$

and

$$\psi_2^\dagger\psi_4 = if(r)g(r)\sqrt{\frac{\ell - m + \frac{1}{2}}{2\ell + 1}}\sqrt{\frac{\ell + m + \frac{3}{2}}{2\ell + 3}}Y_{\ell,m+\frac{1}{2}}(\theta,\phi)^*Y_{\ell+1,m+\frac{1}{2}}(\theta,\phi). \tag{50}$$

Both $\psi_1^\dagger\psi_3$ and $\psi_2^\dagger\psi_4$ are imaginary since the phases of the spherical harmonics cancel, implying that $j_z = 0$. This is also the case for $j = \ell - \frac{1}{2}$. Therefore, in all cases, motion of the electron is constrained to planes of constant z. While this is a simple result, it applies to all hydrogen eigenstates of the forms (46) and (47) and is therefore of general interest.

We find the other components of the current in a similar fashion. For the $j = \ell + \frac{1}{2}$ case,

$$\frac{1}{c}j_x = 2\sin\phi f(r)g(r)\left(\sqrt{\tfrac{\ell-m+1/2}{2\ell+1}}\sqrt{\tfrac{\ell-m-1/2}{2\ell-1}}P_{\ell,m-1/2}P_{\ell+1,m+1/2}\right.$$

$$\left. + \sqrt{\tfrac{\ell-m+1/2}{2\ell+1}}\sqrt{\tfrac{\ell-m+3/2}{2\ell+3}}P_{\ell,m+1/2}P_{\ell+1,m-1/2}\right). \tag{51}$$

We define $F(\cos\theta)$ to be the quantity in brackets, so that

$$\frac{1}{c}j_x = 2\sin\phi f(r)g(r)F(\cos\theta). \tag{52}$$

Because of its similarity in form, j_y also has the $F(\cos\theta)$ term:

$$\frac{1}{c}j_y = -2\cos\phi f(r)g(r)F(\cos\theta). \tag{53}$$

From (3) and (7), the motion of the electron in a plane of constant z is given by the following system of DEs:

$$\begin{aligned} \dot{x} &= \frac{j_x}{\psi^\dagger\psi} = \frac{2cf(r)g(r)F(\cos\theta)\sin\phi}{\psi^\dagger\psi}, \\ \dot{y} &= \frac{j_y}{\psi^\dagger\psi} = \frac{-2cf(r)g(r)F(\cos\theta)\cos\phi}{\psi^\dagger\psi}. \end{aligned} \tag{54}$$

From the polar forms of x and y, we have

$$x\dot{x} + y\dot{y} = \frac{d}{dt}(x^2 + y^2) = 0. \tag{55}$$

In other words, the motion is circular about the z-axis.

A similar proof applies to the $j = \ell - \frac{1}{2}$ case. For the sake of the computations in the next section, the components of the current for this case are $j_z = 0$,

$$\begin{aligned} \frac{1}{c}j_x &= -2\sin\phi f(r)g(r)\Big(\sqrt{\tfrac{\ell-m+1/2}{2\ell+1}}\sqrt{\tfrac{\ell-m-1/2}{2\ell-1}} P_{\ell,m-1/2}P_{\ell-1,m+1/2} \\ &\quad + \sqrt{\tfrac{\ell+m+1/2}{2\ell+1}}\sqrt{\tfrac{\ell+m-1/2}{2\ell-1}} P_{\ell,m+1/2}P_{\ell-1,m-1/2} \Big) \\ &= -2\sin\phi f(r)g(r)G(\cos\theta) \end{aligned} \tag{56}$$

and

$$\frac{1}{c}j_y = 2\cos\phi f(r)g(r)G(\cos\theta), \tag{57}$$

where $G(\cos\theta)$ is the term in brackets in (56). Once again we find that motion about the z-axis is circular.

In summary, we have shown that electron trajectories associated with Dirac hydrogen eigenstates are circular, as was the case for Pauli eigenstates. In the next section, we compute some rates of revolution for these trajectories and their nonrelativistic limits.

Finally, note that if m changes from positive to negative, both $F(\cos\theta)$ and $G(\cos\theta)$ simply undergo an overall sign change. This means that the angular rotation simply changes direction, but maintains the same functional form for $m = \pm\frac{1}{2}$, as was the case for the Pauli trajectories.

3.2. Angular Velocities for $n = 1$ and $n = 2$ Dirac Eigenstates

We find the angular rate of revolution in general from (54) using the relation

$$\dot{y} = (r \sin \theta \cos \phi)\dot{\phi}. \tag{58}$$

From (54), it follows that

$$\frac{d\phi}{dt} = -\frac{2cf(r)g(r)F\cos(\theta)}{\psi^\dagger \psi r \sin \theta \cos \phi}. \tag{59}$$

Although this equation is deceptively simple in appearance, the functions $f(r)$, $g(r)$ – and therefore $\psi^\dagger \psi$ – are quite complicated in form. Since we already know the qualitative motion, explicit computations of the rates of revolution for the general case, beyond the result given in (59), are not particularly enlightening.

However, it is enlightening is to examine the nonrelativistic limits of (59) and compare the results to the values computed from the Pauli equation. If the de Broglie-Bohm picture is to give a coherent account of the hydrogen atom, these results must agree. In what follows, we examine the nonrelativistic limits of (59) for the $n = 1$ and $n = 2$ eigenstates. Note that we compute only the positive m value since the angular velocity simply changes sign for negative m.

3.2.1. n=1

In the ground state, we have [1]

$$g(r) = \left(\frac{2}{a}\right)^{3/2} \sqrt{\frac{1 + \epsilon_1}{2\Gamma(2\gamma_1 + 1)}} e^{-\rho_1/2} \rho_1^{\gamma_1 - 1}$$

$$f(r) = -\sqrt{\frac{1 - \epsilon_1}{1 + \epsilon_1}} g = -\delta g, \tag{60}$$

where

$$\gamma_1 = \sqrt{1 - \alpha^2}, \quad \rho_1 = 2r/a, \quad \epsilon_1 = \left(1 + \frac{\alpha^2}{\gamma_1^2}\right)^{-1/2}, \quad \delta = \sqrt{\frac{1 - \epsilon_1}{1 + \epsilon_1}}, \tag{61}$$

α is the fine structure constant, and a is the Bohr radius. The ground state wave function is given by

$$\psi_1 = \frac{g}{\sqrt{4\pi}}, \quad \psi_2 = 0, \quad \psi_3 = -\frac{1}{\sqrt{4\pi}}if\cos\theta, \quad \psi_4 = -\frac{1}{\sqrt{4\pi}}if\sin\theta e^{i\phi}. \tag{62}$$

This gives

$$\rho = \psi^\dagger \psi = \frac{1}{4\pi}(1 + \delta^2)g^2 \quad \text{and} \quad F(\cos\theta) = \frac{1}{4\pi}\sin\theta. \qquad (63)$$

Substitution into (59) yields, after cancellation,

$$\frac{d\phi}{dt} = \left(\frac{2}{r}\right)\frac{\delta c}{1 + \delta^2}. \qquad (64)$$

In the nonrelativistic limit, $c \to \infty$, which implies that $\alpha = e^2/\hbar c \to 0$ and $\gamma_1 \to 1$. Furthermore, this implies that $\epsilon_1 \to 1$ and $\delta \to 0$. In order to determine the behaviour of δc, we expand ϵ_1 as

$$\epsilon_1 \approx 1 - \frac{1}{2}\left(\frac{\alpha^2}{\gamma_1^2}\right) \qquad (65)$$

so that

$$\frac{1 - \epsilon_1}{1 + \epsilon_1} \to \frac{1}{4}\alpha^2 \quad \text{as} \quad c \to \infty. \qquad (66)$$

Therefore $\delta \to \frac{1}{2}\alpha$. Substitution into (64) yields

$$\frac{d\phi}{dt} \to \frac{1}{r}\alpha c = \frac{e^2}{r\hbar}, \qquad (67)$$

which, when written in terms of the Bohr radius a, becomes

$$\frac{d\phi}{dt} = \frac{\hbar}{m_e a r}. \qquad (68)$$

This is the angular rotation rate for the ground state Dirac wave function. It is in agreement with the Schrödinger rate given by Holland [10], and it is also in agreement with the rate found for the Pauli equation in Table 1.

3.2.2. n=2

1. $2S_{1/2}$ $(n = 2, \quad \ell = 0, \quad j = \frac{1}{2}, \quad m = \frac{1}{2})$

As in the $1s$ case, we have the wave function

$$\psi_1 = \frac{g}{\sqrt{4\pi}}, \quad \psi_2 = 0, \quad \psi_3 = -\frac{1}{\sqrt{4\pi}}if\cos\theta, \quad \psi_4 = -\frac{1}{\sqrt{4\pi}}if\sin\theta e^{i\phi}, \qquad (69)$$

where the functions $f(r)$ and $g(r)$ are suitably modified for the $n = 2$ case. Again, their exact functional form is not relevant, but the relationship between f and g is important; here, rather than (61), we have

$$\rho_2 = \frac{2r}{N_2 a}, \quad N_2 = \sqrt{2(1 + \gamma_1)},$$
$$\epsilon_2 = \left(1 + (\frac{\alpha}{1 + \gamma_1})^2\right)^{-1/2}, \quad \delta = \sqrt{\frac{1 - \epsilon_2}{1 + \epsilon_2}} A, \tag{70}$$

and the number A is given by

$$A = \frac{(2\gamma_1 + 1)(N_2 + 2) - (N_2 + 1)\rho_2}{(2\gamma_1 + 1)N_2 - (N_2 + 1)\rho_2}. \tag{71}$$

After some cancellation, substitution of the wave function into (59) gives, as in (64),

$$\frac{d\phi}{dt} = \left(\frac{2}{r}\right)\frac{\delta c}{1 + \delta^2}. \tag{72}$$

Once again, we examine how the quantities in (70) behave in the nonrelativistic limit $c \to \infty$. In this case,

$$\epsilon_2 \approx 1 - \frac{1}{2}(\frac{\alpha}{1 + \gamma_1})^2, \tag{73}$$

so that

$$\sqrt{\frac{1 - \epsilon_2}{1 + \epsilon_2}} \to \frac{\alpha}{4}. \tag{74}$$

From the properties $\gamma_1 \to 1$, hence $N_2 \to 2$, the limit of A in (70) is

$$A \to \frac{4 - \rho_2}{2 - \rho_2}. \tag{75}$$

This implies that

$$\delta c \to \alpha c \frac{4 - \rho_2}{4(2 - \rho_2)}, \tag{76}$$

and (72) becomes

$$\frac{d\phi}{dt} = \frac{e^2(4 - \rho_2)}{2\hbar r(2 - \rho_2)}, \tag{77}$$

which can be rewritten as

$$\frac{d\phi}{dt} = \frac{\hbar}{2m_e ar} \left(1 - \frac{1}{\frac{r}{2a} - 1} \right). \tag{78}$$

This is the angular rotation rate for the $2s$ Schrödinger state given in [5] and is also in agreement with the Pauli result of Table 1.

2. $2P_{3/2}$ $(n = 2, \quad \ell = 1, \quad j = \frac{3}{2}, \quad m = \frac{3}{2})$

In this case the wave function is given by

$$\psi_1 = \sqrt{\frac{3}{8\pi}} g \sin \theta e^{i\phi}, \quad \psi_2 = 0,$$
$$\psi_3 = -if\sqrt{\frac{3}{8\pi}} \cos \theta \sin \theta e^{i\phi}, \psi_4 = -if\sqrt{\frac{3}{8\pi}} \sin^2 \theta e^{3i\phi}. \tag{79}$$

The functions f and g, and the relationship between them, will be the same as in the above case, because only m has changed. However, we now have $\psi^\dagger \psi = \frac{3}{8\pi} \sin^2 \theta g^2$ in the limit as $\delta \to 0$. Therefore, the expression corresponding to (64) is

$$\frac{d\phi}{dt} = \frac{-2c\delta}{r}. \tag{80}$$

Substitution of the nonrelativistic limiting expressions from the previous case yields

$$\frac{d\phi}{dt} = \frac{\hbar}{2m_e ar}. \tag{81}$$

This is the angular rotation rate for the $2p_1$ Schrödinger state given in [5] and is also in agreement with the Pauli result in Table 1.

3. $2P_{1/2}$ $(n = 2, \quad \ell = 1, \quad j = \frac{1}{2}, \quad m = \frac{1}{2})$

This case is similar to the previous one although the functional forms of f and g are different. We have

$$\psi_1 = \frac{1}{\sqrt{4\pi}} g \cos \theta, \quad \psi_2 = \frac{1}{\sqrt{4\pi}} g \sin \theta e^{i\phi}, \quad \psi_3 = -\frac{if}{\sqrt{4\pi}}, \quad \psi_4 = 0, \tag{82}$$

and

$$\frac{d\phi}{dt} = \left(\frac{2}{r}\right)\frac{\delta c}{1+\delta^2}; \tag{83}$$

and most of the definitions of (70) remain the same. In this case, the term A is given by

$$A = \frac{(2\gamma_1 + 1)N_2 - (N_2 - 1)\rho_2}{(2\gamma_1 + 1)(N_2 - 2) - (N_2 - 1)\rho_2}. \tag{84}$$

In the non-relativistic limit,

$$A \to \frac{6 - \rho_2}{-\rho_2}, \tag{85}$$

so that

$$\frac{d\phi}{dt} = -\frac{\hbar}{m_e r^2}\left(3 - \frac{r}{2a}\right). \tag{86}$$

In this case, no comparison can be made with any Schrödinger state.

4. $2P_{3/2}$ $(n = 2, \quad \ell = 1, \quad j = \frac{3}{2}, \quad m = \frac{1}{2})$

This case is somewhat different. Here, the wave function is

$$\psi_1 = \frac{1}{\sqrt{2\pi}}g\cos\theta, \quad \psi_2 = -\frac{1}{\sqrt{8\pi}}g\sin\theta e^{i\phi},$$

$$\psi_3 = -if\frac{1}{\sqrt{8\pi}}(3\cos^2\theta - 1), \quad \psi_4 = -if\sqrt{\frac{9}{8\pi}}\sin\theta\cos\theta e^{i\phi}, \tag{87}$$

and

$$\psi^\dagger\psi = \frac{1}{8\pi}(4\cos^2\theta + \sin^2\theta)g^2 + \frac{1}{8\pi}((3\cos^2\theta - 1)^2 + 3\sin^2\theta\cos^2\theta)f^2. \tag{88}$$

Furthermore, the function $F(cos\theta)$ becomes

$$F(cos\theta) = \frac{1}{8\pi}\sin\theta(8\cos^2\theta - \sin^2\theta). \tag{89}$$

Again, $f = -\delta g$, with

$$\delta = \sqrt{\frac{1 - \epsilon_3}{1 + \epsilon_3}}, \quad \epsilon_3 = \left(1 + \frac{\alpha^2}{\gamma_2^2}\right)^{-1/2}, \quad \gamma_2 = \sqrt{4 - \alpha^2}, \quad (90)$$

and we find from (59) that

$$\frac{d\phi}{dt} = \frac{2\delta c(8\cos^2\theta - \sin^2\theta)}{r(4\cos^2\theta + \sin^2\theta)}. \quad (91)$$

As $c \to \infty$,

$$\epsilon_3 \approx 1 - \frac{1}{2}\left(\frac{\alpha}{2}\right)^2, \quad (92)$$

so that $\delta c \to \frac{\alpha}{4}$. After substituting and rewriting α, we obtain

$$\frac{d\phi}{dt} = \frac{\hbar}{2m_e ar}\left(\frac{8\cos^2\theta - \sin^2\theta}{4\cos^2\theta + \sin^2\theta}\right). \quad (93)$$

Once again, no comparison can be made with any Schrödinger state.

In each case presented above, the nonrelativistic limit of the Dirac angular velocity agrees with the corresponding Pauli result given in Table 1. We expect this, since the Pauli equation is the nonrelativistic limit of the Dirac equation. However, the results are not obvious, since the expressions in (7) and (10) for, respectively, the Dirac and Pauli currents are quite different.

4. CONCLUDING REMARKS

In this paper, we have determined the general features of de Broglie-Bohm trajectories for energy/total angular momentum eigenstates of the Pauli and Dirac hamiltonians for hydrogen. In all cases, the electron, assumed to be in an eigenstate of M_z, the z-component of the total angular momentum, M, is confined to a plane of constant z-value and executes circular motion about the z-axis with a constant angular velocity $d\phi/dt$. As well, we have outlined a procedure to compute these angular velocities for general eigenstates and have explicitly computed them for the $n = 1$ and $n = 2$ Pauli and Dirac hydrogen eigenstates.

In the cases where the Pauli eigenstates are also eigenstates of the s_z operator, our results from the Pauli equation agree with earlier computations of the trajectories of corresponding Schrödinger eigenstates [5]. Furthermore, the nonrelativistic limits of the Dirac results agree with the Pauli results. We have therefore shown that the de

Broglie-Bohm causal picture can be applied coherently to the hydrogen atom, moving from the Schrödinger to the Pauli and ultimately to the Dirac equation.

Finally, one may well wish to consider trajectories for Pauli or Dirac wave functions other than those considered in this paper. For example, it may be interesting to examine trajectories for particular linear combinations of eigenstates. (In [5], we examined Bohm trajectories for the familiar Schrödinger $2p_x$ and $2p_y$ orbitals used in descriptions of chemical bonding. As well, we examined trajectories associated with a time-varying linear combination of $1s$ and $2p_0$ hydrogenic wave functions that simulated an electronic transition induced by an oscillating electric field.) The method of computing Bohm trajectories outlined in Sections 2 and 3 can be extended in a straightforward manner to treat such linear combinations, although the computations may well become quite complicated.

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