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Spin-dependent Bohm trajectories for hydrogen eigenstates

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Abstract

The Bohm trajectories for several hydrogen atom eigenstates are determined, taking into account the additional momentum term $\nabla\rho \times \mathbf{s}$ that arises from the Pauli current. Unlike the original Bohmian result, the spin-dependent term yields nonstationary trajectories. The relationship between the trajectories and the standard visualizations of orbitals is discussed. The trajectories for a model problem that simulates a $1s2p$ transition in hydrogen are also examined.

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1. Introduction

In Bohm's original causal interpretation of quantum mechanics [1], the motion of a quantum mechanical particle is determined by its wavefunction ψ, which acts as a guidance wave [3]. If the wavefunction is written as

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

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

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

The *Schrödinger current* associated with ψ is given by

$$\mathbf{j} = \frac{1}{m}\rho\mathbf{p}, \tag{3}$$

where $\rho = \psi^*\psi = R^2$. Comprehensive discussions of this causal interpretation of quantum mechanics can be found in [2] and [7].

However, as Holland [8] has pointed out, Eqs. (2) and (3) are relevant only to spin-0 particles. For particles with spin, these equations are inconsistent if the theory is to be ultimately embedded in a relativistic theory. 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 [8]

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

In a number of earlier works, including [4–6], the current vector associated with Eq. (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*, as opposed to Eq. (3), the

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nonrelativistic limit of the *Gordon current*. (In these papers, it was claimed that consistency with Dirac theory requires that Schrödinger theory be regarded as describing an electron in an eigenstate of spin.) The spin-dependent term was also discussed in [2] but only in the context of the Pauli equation and not the Schrödinger equation.

The momentum defined in Eq. (2) predicts that electrons in an eigenstate are stationary since $\nabla S = 0$. This is a counterintuitive result of Bohm's original theory, but one which no longer persists when the extra term in (4) is taken into account. For example, consider an electron in the $1s$ ground eigenstate of hydrogen,

$$\psi_{100} = \frac{1}{\sqrt{\pi a^3}} e^{-r/a}, \tag{6}$$

where $a = \hbar^2/(me^2)$ is the Bohr radius. Also assume that the electron is in a definite spin eigenstate: without loss of generality, let its spin vector be given by $\mathbf{s} = \frac{\hbar}{2}\mathbf{k}$. (We shall justify this assumption below.) Holland [7] showed that the extra term $\nabla \log \rho \times \mathbf{s}$ implies that the polar coordinates r and θ are constant, with angle ϕ evolving in time as follows:

$$\frac{d\phi}{dt} = \frac{\hbar}{mar}. \tag{7}$$

All points on a sphere of radius r orbit the z-axis at the same rate. If $r = a$, the angular frequency is on the order of 10^{16} s^{-1}, cf. Eq. (32).

In Section 2, we examine the effects of the extra term in (4) for an electron in several eigenstates of the hydrogen atom. Because the momentum equation (4) now involves spin, a complete description of the electron in the atom—provided by an appropriate wavefunction—will have to involve both spatial as well as spin information. Let us denote the complete wavefunction of the electron by $\Psi(\mathbf{x}, \mathbf{s}, t)$, where $\mathbf{s}$ denotes appropriate spin coordinates. Since the hamiltonian describing the evolution of Ψ is the simple spin-independent hydrogen atom hamiltonian $\widehat{H}_0$, we may write Ψ as the tensor product $\psi(\mathbf{x}, t)\zeta(\mathbf{s})$, where $\psi(\mathbf{x}, t)$ is a solution of the time-dependent Schrödinger equation,

$$i\hbar \frac{\partial \psi}{\partial t} = \widehat{H}_0 \psi, \tag{8}$$

and $\zeta(\mathbf{s})$ is an eigenfunction of the commuting spin operators $\hat{S}^2$ and $\hat{S}_z$, with $\hat{S}^2\zeta = \frac{3}{4}\hbar\zeta$ and $\hat{S}_z\zeta = \frac{1}{2}\hbar\zeta$. Thus ζ defines the "alpha" or "spin up" state to which corresponds the spin vector $\mathbf{s} = \frac{\hbar}{2}\mathbf{k}$. As such, the remainder of our discussion can focus on the evolution of the spatial portion of the wavefunction $\psi(\mathbf{x}, t)$. In the parlance of "state preparation", one can view this construction as preparing the electon with constant spin vector $\mathbf{s}$ and initial wavefunction $\psi(\mathbf{x}, 0)$. Given an initial position $\mathbf{x}_0$ of the electron, Eq. (4) will then determine its initial momentum $\mathbf{p}_0$, from which its causal trajectory then evolves.

In Section 3, we examine the trajectories of an electron, as dictated by Eq. (4), where ψ is a linear combination of $1s$ and $2p_0$ eigenstates evolving in time under the hydrogen atom hamiltonian, cf. Eq. (8). Once again because of the spin-independence of $\widehat{H}_0$, we may assume that the spin vector of the electron is constant, i.e., $\mathbf{s} = \frac{\hbar}{2}\mathbf{k}$, and thereby focus on the time evolution of the spatial wavefunction $\psi(\mathbf{x}, t)$. This simple model was chosen to determine the major qualitative features of Bohmian trajectories for a $1s2p$ transition induced by an oscillating electric field. We have analyzed trajectories corresponding to the time-dependent wavefunction associated with the transition hamiltonian and shall report the results elsewhere.

2. Spin-dependent trajectories of electrons in hydrogen eigenstates

2.1. Qualitative features

Following the discussion at the end of the previous section, we consider an electron with spin vector $\mathbf{s}$ that begins in a hydrogenic eigenstate, i.e., $\psi(\mathbf{x}, 0) = \psi_{nlm}(\mathbf{x})$. The time evolution of the spatial wavefunction is simply

$$\psi(\mathbf{x}, t) = \psi_{nlm}(\mathbf{x}) e^{-iE_n t/\hbar}. \tag{9}$$

Comparing Eqs. (9) and (1), we see that $\nabla S = 0$ so that the momentum in Eq. (4) is given by

$$\mathbf{p} = \nabla \log \rho \times \mathbf{s}. \tag{10}$$

Some simple qualitative information about the electron trajectories is readily found from this equation. First, the vector $\nabla \log \rho$ points in the direction of the steepest increase in $\log \rho$, hence in $\rho = |\psi|^2$. Because of the cross product, the momentum vector $\mathbf{p}$ is perpendicular to this direction. In other words, the tra-

jectories of the electron lie on level surfaces of $|\psi|^2$. However, **p** is also perpendicular to the direction of the spin, assumed to lie along the z-axis in this discussion. This implies that z is constant for these Bohm trajectories.

From the above analysis, the *shape* of the Bohm trajectories may be found by computing level surfaces of $|\psi|^2$—or simply ψ for real-valued eigenfunctions—and then finding the intersections of these surfaces with planes of constant z. An electron in the $1s$ state of hydrogen, cf. Eq. (6), must therefore execute a circular orbit about the z-axis. However, the angular velocity of this orbit, cf. Eq. (7), cannot be determined from this analysis.

For the $2s$ case, with quantum numbers $(n, l, m) = (2, 0, 0)$, the wavefunction is given by

$$\psi_{200} = \frac{1}{\sqrt{32\pi a^5}}\left(1 - \frac{r}{2a}\right)e^{-r/2a}. \tag{11}$$

The level surfaces of ψ_{200} are spheres whose intersection with planes of constant z are circles (with constant θ values). The electron again travels about the z-axis in a circular orbit.

In the $2p_0$ case, $(n, l, m) = (2, 1, 0)$, the wavefunction is given by

$$\psi_{210} = \frac{1}{\sqrt{32\pi a^5}} re^{-r/2a}\cos\theta. \tag{12}$$

The condition that both ψ and z be constant is satisfied only if both r and θ are constant, once again yielding circular orbits about the z-axis.

In the other $2p$ cases, $(n, l, m) = (2, 1, \pm 1)$, the wavefunctions are given by

$$\psi_{21(\pm1)} = \mp\frac{1}{\sqrt{32\pi a^5}} re^{-r/2a}\sin\theta e^{\pm i\phi}. \tag{13}$$

The condition $\rho = |\psi|^2 = \text{constant}$ yields a relation $r = r(\theta)$ defined implicitly by

$$\sin\theta = \frac{K}{r}e^{r/2a}, \tag{14}$$

where K is a constant. Since $z = r\cos\theta$ is also constant, it follows that both r and θ are constants of motion so that there is circular motion about the z-axis.

2.2. More detailed dynamical descriptions of the trajectories

For more complicated hydrogen eigenstates (see below), it may not be as simple to find closed form expressions for level sets of $|\psi|^2$ so that the method of qualitative analysis outlined above may be difficult if not impossible. As well, it is desirable to extract quantitative information such as the angular velocity $d\phi/dt$ of the circular orbits deduced earlier. We therefore analyze the differential equations of motion defined by Eq. (10).

The gradient term from Eq. (10) is given by

$$\nabla\log\rho = \nabla\log\psi^*\psi = 2\,\mathrm{Re}\left(\frac{(\nabla\psi)\psi^*}{\psi\psi^*}\right). \tag{15}$$

For real wavefunctions, this simplifies to

$$\nabla\log\rho = 2\frac{\nabla\psi}{\psi}. \tag{16}$$

In spherical polar coordinates (r, θ, ϕ), the spin vector $\mathbf{s} = \frac{\hbar}{2}\mathbf{k}$ is given by $\mathbf{s} = \frac{\hbar}{2}(\cos\theta\hat{r} - \sin\theta\hat{\theta})$. It is convenient to compute the cross product in the (right-handed) spherical polar coordinate system:

$$\mathbf{A}\times\mathbf{B} = \begin{vmatrix} \hat{\theta} & \hat{\phi} & \hat{r} \\ A_\theta & A_\phi & A_r \\ B_\theta & B_\phi & B_r \end{vmatrix}. \tag{17}$$

For the $1s$ ground state defined in Eq. (6), $\nabla\psi = -\frac{1}{a}\psi\hat{r}$. Thus

$$\mathbf{p} = \frac{\hbar}{a}\sin\theta\hat{\phi}. \tag{18}$$

Since $p_r = p_\theta = 0$, it follows that r and θ are constant, implying that z is constant, i.e., circular orbits about the z-axis. Holland's result in Eq. (7) follows.

For the $2s$ wavefunction defined in Eq. (11),

$$\frac{\nabla\psi_{200}}{\psi_{200}} = -\frac{1}{2a}\left[\frac{1}{1-\frac{r}{2a}} + 1\right]\hat{r}, \tag{19}$$

so that

$$\mathbf{p} = -\frac{\hbar}{2a}\sin\theta\left[\frac{1}{1-\frac{r}{2a}} + 1\right]\hat{\phi}. \tag{20}$$

Once again r and θ are constant. From the relation $d\phi/dt = p_\phi/mr\sin\theta$, we have

$$\frac{d\phi}{dt} = -\frac{\hbar}{2mar}\left[\frac{1}{\frac{r}{2a}-1} - 1\right]. \tag{21}$$

Note that the pole at $r = 2a$ coincides with the zero of the $2s$ wavefunction, implying that the probability of finding the electron at $r = 2a$ is zero. Also note that (i) $\dot{\phi} > 0$ for $0 < r < 2a$, (ii) $\dot{\phi} < 0$ for $2a < r < 3a$, (iii) $\dot{\phi} = 0$ for $r = 3a$ and (iv) $\dot{\phi} > 0$ for $r > 3a$. For $r = a$, the angular velocity $\dot{\phi}$ is equal to that of the $1s$ ground state, cf. Eq. (7).

For the $2p_0$ state defined in Eq. (12),

$$\frac{\nabla\psi_{210}}{\psi_{210}} = \frac{1}{r}\left(1 - \frac{r}{2a}\right)\hat{r} - \frac{\sin\theta}{r\cos\theta}\hat{\theta}. \tag{22}$$

From Eq. (10),

$$\mathbf{p} = \frac{\hbar\sin\theta}{2a}\hat{\phi}, \tag{23}$$

implying that

$$\frac{d\phi}{dt} = \frac{\hbar}{2mar}. \tag{24}$$

This is one-half the angular velocity for the $1s$ ground state.

For the $2p$ states with $m = \pm 1$, cf. Eq. (13), the spherical symmetry has been lost and we find that

$$\mathbf{p} = -\frac{\hbar}{r}\left[\sin\theta\left(1 - \frac{r}{2a}\right) + \frac{\cos^2\theta}{\sin\theta}\right]\hat{\phi}. \tag{25}$$

Once again, r and θ are constant, implying circular orbits about the z-axis. However the orbital angular velocity depends upon r and θ in a more complicated fashion:

$$\frac{d\phi}{dt} = \frac{\hbar}{mr^2}\left[\frac{r}{2a} - 1 - \cot^2\theta\right]. \tag{26}$$

For $\theta = \pi/2$, i.e., the xy plane, $\dot{\phi} = 0$ for $r = 2a$. This implies that there is a ring of equilibrium points on the xy plane at which the electron is stationary. For all other nonzero r values on the xy plane the electron revolves about the z-axis: $\dot{\phi} < 0$ for $0 < r < 2a$ and $\dot{\phi} > 0$ for $r > 2a$. A ring of stationary points exists on every plane parallel to the xy plane: for any fixed $\theta_0 \in (0, \pi/2)$, the ring is determined by the relation $r = 2a\csc^2\theta_0$. The radius of this ring (distance from the z-axis) is $r\sin\theta_0 = 2a/\sin\theta_0$. The set of all points at which the electron is stationary defines a surface that is generated by revolving the curves

$$z = \pm x\left[\left(\frac{x}{2a}\right)^2 - 1\right]^{1/2}, \quad x \geqslant 2a, \tag{27}$$

about the z-axis. In the region between this surface and the z-axis, $\dot{\phi} < 0$; on the other side of this surface, $\dot{\phi} > 0$.

In summary, for each of the hydrogen eigenstates studied above, the Bohm trajectories are circular orbits about the z-axis, the assumed orientation of the electron spin vector **s**. Furthermore, the quantitative behaviour of the angular velocity has been determined in all cases.

We now examine Bohm trajectories for the real hydrogen wavefunctions, [9]

$$\begin{aligned}\psi_{2p_x} &= Nre^{-r/2a}\sin\theta\cos\phi,\\ \psi_{2p_y} &= Nre^{-r/2a}\sin\theta\sin\phi,\end{aligned} \tag{28}$$

where $N = 1/\sqrt{32\pi a^5}$. The probability distributions associated with these wavefunctions are the familiar hydrogen orbitals used in descriptions of organic chemical bonding.

The ψ_{2p_x} and ψ_{2p_y} wavefunctions are obtained by appropriate linear combinations of the energetically degenerate eigenfunctions $\psi_{21(\pm 1)}$ of Eq. (13). Therefore they are also eigenfunctions of the hydrogen atom hamiltonian $\widehat{H}_0$ with energy E_2. From Eq. (9), it follows that $\nabla S = 0$. The cross product of Eq. (10) has components in all three variables, resulting in a system of three coupled ordinary differential equations which must be integrated to find the trajectories.

The system of ODEs associated with the ψ_{2p_x} wavefunction is given by

$$\begin{aligned}\frac{dr}{dt} &= -\frac{\hbar}{mr}\tan\phi,\\ \frac{d\theta}{dt} &= -\frac{\hbar}{mr^2}\cot\theta\tan\phi,\\ \frac{d\phi}{dt} &= -\frac{\hbar}{mr^2}\left(1 - \frac{r}{2a} + \cot^2\theta\right).\end{aligned} \tag{29}$$

Note that the ϕ DE is identical to Eq. (25). From the first two DEs, we have

$$\frac{dr}{d\theta} = r\tan\theta, \tag{30}$$

which is easily integrated to give $z = r\cos\theta = C$, in agreement with our earlier analysis. It follows that r and θ are constant when $\phi = 0$ or π. If $\theta = \pi/2$ as well, then $\dot{\phi} = 0$ for $r = 2a$, implying the existence of two equilibrium points at $(x, y, z) = (2a, 0, 0)$ and $(-2a, 0, 0)$. At these points, the electron is stationary.

In fact, these are two particular cases of an infinity of equilibrium points that are given by the conditions $\phi = 0, \pi$ (xz plane) and

$$1 - \frac{r}{2a} + \cot^2\theta = 0. \tag{31}$$

By virtue of the above relation and Eq. (25), the equilibrium points of this system lie on the two curves defined by Eq. (27) in the xz plane as well as their reflections about the z-axis. Each of these points corresponds to the points of highest and lowest "elevation" (from the horizontal xy plane) of the familiar dumb-belled level surfaces $\rho = \psi^2 = C$ of the orbital. At all of these points, the electron is stationary.

The system of ODEs in (29) may be integrated numerically. However, it is useful to introduce the dimensionless variables $\xi = r/a$ and $\tau = \omega_0 t$, where

$$\omega_0 = \frac{E_2 - E_1}{\hbar} = \frac{3\hbar}{8ma^2} \tag{32}$$

is the angular frequency associated with the $n = 1$ to $n = 2$ transition in the hydrogen atom ($\omega_0 \approx 1.549 \times 10^{16}\ \mathrm{s}^{-1}$). The scaled equations become

$$\begin{aligned}
\frac{d\xi}{d\tau} &= -\frac{8}{3\xi}\tan\phi, \\
\frac{d\theta}{d\tau} &= -\frac{8}{3\xi^2}\cot\theta\tan\phi, \\
\frac{d\phi}{d\tau} &= -\frac{8}{3\xi^2}\left(1 - \frac{\xi}{2} + \cot^2\theta\right).
\end{aligned} \tag{33}$$

Fig. 1 shows the numerically integrated trajectories for several initial conditions in the xz plane. Note that there is a good qualitative agreement between these trajectories and the orbital shapes of the $2p_x$ state as depicted in textbook contour plots. (No orbits cross the yz plane since it is a nodal surface.) The numerical results confirm that motion is periodic. Angular frequency values are observed to be of the order of ω_0. These periodic orbits are stable in the sense of Lyapunov.

The nondimensional and numerical analysis of the $2p_y$ case proceeds in a similar fashion. The resulting system of ODEs represents a rotation of the system in Eq. (29) by an angle of $\pi/2$ in ϕ.

To summarize this section, we have shown that the spin-dependent Bohm trajectories for the ground and first excited states of the hydrogen atom are stable periodic orbits. There are no exceptional orbits that deviate from this regularity. For some of the $2p$ states, these orbits include families of stationary points that have zero Lebesgue measure in $\mathbf{R}^3$. These results are intuitively more acceptable than the original Bohmian result that *all* trajectories associated with a given eigenstate are stationary.

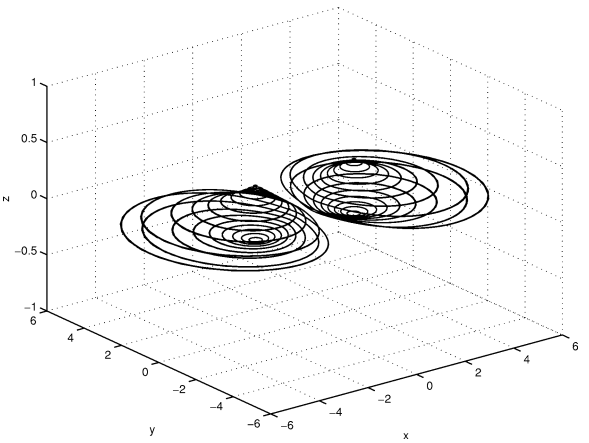

Fig. 1. Spin-dependent Bohm trajectories for the $2p_x$ hydrogen eigenstate.

3. Trajectories associated with a linear superposition of hydrogenic eigenfunctions

We now examine the Bohm trajectories of an electron with constant spin vector $\mathbf{s} = \frac{\hbar}{2}\mathbf{k}$ but with a spatial wavefunction $\psi(\mathbf{x}, t)$ that begins as a linear combination of $1s$ and $2p_0$ hydrogenic eigenfunctions,

$$\psi(\mathbf{x}, 0) = c_1\psi_{100}(\mathbf{x}) + c_2\psi_{210}(\mathbf{x}), \tag{34}$$

where $c_1^2 + c_2^2 = 1$. (The assumption that the electron is in a well-defined "spin up" eigenstate was justified at the end of Section 1.)

The time evolution of this spatial wavefunction, as dictated by the time-dependent Schrödinger equation (8), will be given by

$$\psi(\mathbf{x}, t) = c_1\psi_{100}(\mathbf{x})e^{-iE_1t/\hbar} + c_2\psi_{210}(\mathbf{x})e^{-iE_2t/\hbar}. \tag{35}$$

This linear combination was chosen in order to examine some of the qualitative features of the trajectories associated with the $1s2p_0$ transition in hydrogen induced by an oscillating electric field of the form $\hat{z}E_0\cos\omega t$. Indeed, many of the qualitative features of

this problem are captured by this model, with the exception of additional oscillations along invariant surfaces due to the oscillating field. We have studied the trajectories of this transition problem in detail and shall report the results elsewhere.

The wavefunction in Eq. (35) is *not* a linear combination of energetically degenerate states. As such ∇S, the first term of the momentum in Eq. (4), is nonzero. It can be computed as follows:

$$\nabla S = \frac{\hbar}{\psi^*\psi}\,\mathrm{Im}[(\nabla\psi)\psi^*]. \tag{36}$$

The results are

$$\begin{aligned} p_r &= -\frac{\hbar}{\psi^*\psi}c_1c_2N_1N_2e^{-3r/2a} \\ &\quad\times\cos\theta\sin\omega_0 t\left(1+\frac{r}{2a}\right), \\ p_\theta &= \frac{\hbar}{\psi^*\psi}c_1c_2N_1N_2e^{-3r/2a}\sin\theta\sin\omega_0 t, \\ p_\phi &= 0. \end{aligned} \tag{37}$$

Here, N_1 and N_2 denote, respectively, the normalization factors of the $1s$ and $2p$ states and ω_0 is defined in Eq. (32). This is the momentum of the original Bohmian formulation $\mathbf{p} = \nabla S$. The angle ϕ is constant, implying that there is no orbital motion about the z-axis.

The second term in the momentum equation (4) contributes only to the ϕ-momentum:

$$p_\phi = -\frac{\hbar}{\psi^*\psi}[Y\cos\theta + X\sin\theta], \tag{38}$$

where

$$\begin{aligned} X &= -\frac{1}{a}c_1^2N_1^2e^{-2r/a} + c_2^2N_2^2r\left(1-\frac{r}{2a}\right)e^{-r}\cos^2\theta \\ &\quad + c_1c_2N_1N_2\left(1-\frac{3r}{2a}e^{-3r/2a}\right)\cos\theta\cos\omega_0 t, \\ Y &= -c_2^2N_2^2re^{-r}\sin\theta\cos\theta \\ &\quad - c_1c_2N_1N_2e^{-3r/2a}\sin\theta\cos\omega_0 t. \end{aligned} \tag{39}$$

(The terms X and Y are the r and θ components, respectively, of $\nabla\log\psi^*\psi$.) Once again, the spin-dependent momentum term implies orbital motion about the z-axis.

The p_r and p_θ equations of (37) along with p_ϕ in (38) yield differential equations in the coordinates r, θ and ϕ. Once again, we rewrite these DEs in terms of the dimensionless variables $\xi = r/a$ and $\tau = \omega_0 t$. The net result is the following system:

$$\begin{aligned} \frac{d\xi}{d\tau} &= -\frac{\sqrt{2}}{3D}c_1c_2\left(1+\frac{\xi}{2}\right)e^{-3\xi/2}\cos\theta\sin\tau, \\ \frac{d\theta}{d\tau} &= \frac{\sqrt{2}}{3D\xi}c_1c_2e^{-3\xi/2}\sin\theta\sin\tau, \\ \frac{d\phi}{d\tau} &= \frac{8}{3D\xi}\left[c_1^2e^{-2\xi} + \frac{1}{64}c_2^2\xi^2e^{-\xi}\cos^2\theta\right. \\ &\qquad \left. + \frac{3}{8\sqrt{2}}c_1c_2\xi e^{-3\xi/2}\cos\theta\cos\tau\right], \end{aligned} \tag{40}$$

where

$$\begin{aligned} D &= c_1^2e^{-2\xi} + \frac{1}{32}c_2^2\xi^2e^{-\xi}\cos^2\theta \\ &\quad + \frac{1}{2\sqrt{2}}c_1c_2\xi e^{-3\xi/2}\cos\theta\cos\tau. \end{aligned} \tag{41}$$

We first note the following two special cases for the system of DEs in (40) (the primes denote differentiation with respect to τ):

(1) $(c_1, c_2) = (1, 0)$ ($1s$ state): $\xi' = \theta' = 0$, and $\phi' = 8/(3\xi)$, in agreement with Eq. (7).
(2) $(c_1, c_2) = (0, 1)$ ($2p_0$ state): $\xi' = \theta' = 0$, and $\phi' = 4/(3\xi)$, in agreement with Eq. (24).

In these cases, the trajectories are simple circular orbits about the z-axis, as expected.

More generally, the DEs in ξ and θ are decoupled from the ϕ DE. From the former two DEs, we have

$$\frac{d\xi}{d\theta} = -\xi\left(1+\frac{\xi}{2}\right)\cot\theta. \tag{42}$$

This separable DE is easily solved to give

$$\xi = \frac{2}{A\sin\theta - 1}, \quad A = \frac{2+\xi_0}{\xi_0\sin\theta_0} > 1, \tag{43}$$

where $\xi_0 = \xi(0)$ and $\theta_0 = \theta(0)$. In a plane with $z = \xi\cos\theta$ defining the vertical axis (recall that $0 \leqslant \theta \leqslant \pi/2$), the relation $\xi(\theta)$ defines a family of hyperbolae. The asymptotes of the hyperbola in Eq. (43) are given by the rays $\theta = \theta_1 = \mathrm{Sin}^{-1}[\xi_0\sin\theta_0/(\xi_0+2)]$ and $\theta = \theta_2 = \pi - \theta_1$. If we choose $\theta_0 = \pi/2$ (x-axis), then $\xi_0 \to 0^+$, $\theta_1 \to 0^+$, i.e., the hyperbolae flatten as they approach the z-axis.

Since the ξ-θ DEs are decoupled from the ϕ equation in (40), the electron will remain on the

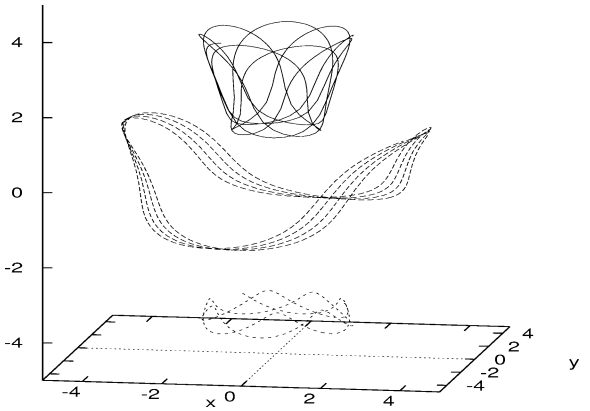

Fig. 2. Spin-dependent Bohm trajectories for the $1s2p_0$ linear combination, $c_1 = c_2 = \frac{1}{\sqrt{2}}$, as computed from Eq. (40), for $0 \leqslant \tau \leqslant 50$.

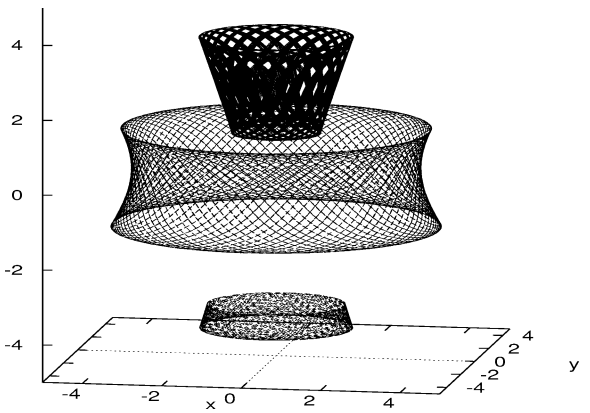

Fig. 3. The spin-dependent Bohm trajectories from Fig. 2, but computed for $0 \leqslant \tau \leqslant 1000$ in order to show the invariant surfaces on which the trajectories lie.

3D surface obtained by rotating the appropriate $\xi(\theta)$ hyperbola in Eq. (43) about the z-axis. In other words, the hyperboloid of revolution is an invariant set in $\mathbf{R}^3$ for the electronic trajectory. Plots of three sample trajectories for the case $c_1 = c_2 = \frac{1}{\sqrt{2}}$ are shown in Fig. 2. The time interval $0 \leqslant \tau \leqslant 50$ was chosen so that the oscillatory nature of the solutions could be seen.

In Fig. 3, the time interval of these solutions has been extended to $0 \leqslant \tau \leqslant 1000$. The invariant surfaces associated with these trajectories can be discerned from the plots.

A more realistic simulation of the oscillating electric field problem is accomplished if we set the coefficients c_1 and c_2 in Eq. (34) to be

$$c_1 = \cos\omega t, \qquad c_2 = \sin\omega t, \quad t \geqslant 0, \tag{44}$$

so that the atom begins in the ground state and proceeds to oscillate between it and the $2p_0$ excited state. In this case, the electron trajectories, as determined by the system of ODEs in (40), will still be constrained to the invariant hyperboloid surfaces of revolution. However, there will be additional oscillatory components in these trajectories due to the periodic behaviour of the c_i in Eq. (44). A detailed examination of the possible qualitative behaviour of solutions is beyond the scope of this letter.

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