Electron Spin in a Quantum Well

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The wave nature of the electron spin proposed earlier [1,2] is studied by solving the Dirac equation with a complete form of 4-spinor. The result shows a stable circulating total current density with a donut shaped topography for the eigenstate electron inside a quantum well. The spin value inside the well is modified by the confining geometry. Our analysis also shows that a free electron Gaussian wavepacket is unstable and experiences quick decoherence. The impacts of the wave spin on quantum computing and quantum information technologies are discussed in principle.

I. INTRODUCTION

Spin is an essential property of an electron that has played a pivotal role in the development of quantum mechanics and quantum field theory [3]. Demonstrated by the well-known Stern-Gerlach experiment [4] exactly a century ago, spin was interpreted first by Uhlenbeck and Goudsmit [5] in 1926 as the internal angular momentum of the spinning particle electron. Since then, the use of the widely accepted 2-spinor \((\begin{array}{c}1 \\ 0 \\ 0 \\ 1 \end{array})\) to represent the electron spin up and down [6] only solidifies the view of an abstract and internal spin of the electron. However, there are some profound obstacles of this view, including that no internal structure of the electron is observed and the electron must spin faster than the speed of light [7].

An alternative view proposed by Belinfante [1] and Ohanian [2] attributes the spin to the electron wave instead. Their works show that the electron momentum and current densities calculated from the quantum mechanical wavefunctions have circulating flow patterns that give rise to the electron spin and magnetic moment. Here the wavefunction satisfies the Dirac equation [3]

\[
\frac{1}{c}\frac{\partial}{\partial t}\psi(x) = (-\alpha \cdot \nabla - i\frac{mc}{\hbar}\gamma^0)\psi(x),
\]

where \(x = (t, \mathbf{r})\) is a four-vector and \(\alpha\) are \(4 \times 4\) matrices representing the spin properties. Any observable quantities calculated from the wavefunction thus carry the spin properties into the space permeated by the wavefunctions beyond the locality of the electron particle. The behavior of the total charge and current density expressed by the four-current \(j = (\rho, \mathbf{j})\)

\[
\begin{align*}
\rho(x) &= e\bar{\psi}(x)\psi(x) \\
\mathbf{j}(x) &= e\bar{\psi}(x)\gamma^\mu\psi(x)
\end{align*}
\]

is of particular interest because it ties to the whole spectrum of electromagnetic phenomena by Maxwell equation

\[
\left(\frac{1}{c^2}\frac{\partial^2}{\partial t^2} - \nabla^2\right)A = \mu_0\mathbf{j},
\]

where \(A = (\phi, \mathbf{A})\) is the electromagnetic four-potential, providing the possibility that the wave nature of the spin can be experimentally measured and verified.

In the original paper [2], a Gaussian wavefunction is used to describe a free electron wavepacket of diameter \(d\), spin up, and zero momentum expectation value

\[
\psi(x) = \left(\frac{2\pi}{d^2}\right)^{-3/2} e^{-\frac{x^2+y^2+z^2}{2d^2}} \begin{pmatrix}1 \\
0 \\
0 \\
0 \end{pmatrix}.
\]

Plugging Eq.4 to Eq.2 yields the Gaussian charge distribution but zero total current density \(\mathbf{j} = 0\). However, the circulating flow of the current density is demonstrated through a spin current density defined as

\[
\mathbf{j}_s = \frac{i\hbar}{2m} \frac{\partial}{\partial t}\bar{\psi}\sigma^k\psi + \frac{i\hbar}{2mc} \frac{\partial}{\partial t} \bar{\psi}\sigma^0\psi
\]

as part of the total current density with the help of the Gordon decomposition

\[
j^k = \frac{i\hbar}{2m} \left[\bar{\psi}(\partial_k\psi) - (\partial_k\bar{\psi})\psi\right] + \frac{i\hbar}{2m} \frac{\partial}{\partial t} \bar{\psi}\sigma^k\psi + \frac{i\hbar}{2mc} \frac{\partial}{\partial t} \bar{\psi}\sigma^0\psi,
\]

where the three terms are the convection, magnetization, and polarization current densities, respectively. The spin current density is the sum of two terms that contain the \(4 \times 4\) matrix \(\sigma\).

The Gordon decomposition provides insights to the wave spin picture, but the appearance of circulating flow in the spin current density but not in the total current density raises the question of whether the wave effect of the spin is internally canceled out and not observable externally.

Settling down the wave or particle nature of the spin is intriguing not only to the physics community but to the general technical communities as well, since, if the wave nature of the spin is correct, the spin may be manipulated and utilized similarly to an optical wave for novel applications. In this paper, we continue the wave spin discussion pioneered by previous authors [1,2,3]. We base on the solutions of the Dirac equation to calculate observable quantities. SI units are adopted for all expressions throughout the paper to facilitate practical calculations. The main physical constants used in the paper are summarized in Table I.
II. DIRAC FREE ELECTRON GAUSSIAN WAVEPACKET

First, we shall point out that the finite-sized wavepacket of Eq. 2 has finite momentum values according to the uncertainty principle \( pd \geq \hbar \), even for a wavepacket with zero momentum expectation. Just as transverse momentums for a Gaussian laser beam balance the momentum conservation in a laser-electron interaction 9, the non-zero momentum due to the finite \( d \) leads to the circulating flow of the total current density as shown in the following.

The solution of the Dirac equation is a vector in the Hilbert space spanned by the eigenstates. The eigenstate according to the uncertainty principle \( \psi \) states of Eq.7, the Dirac equation should be the superposition of eigenstates having different temporal phase factors to cause decoherence in the electron wavepacket.

The solution of the Dirac equation is a vector in the Hilbert space spanned by the eigenstates. The eigenstate as shown in the following.

\[
\psi(x) = e^{-i\frac{\lambda}{2} E_t t + i\frac{\lambda}{2} P \cdot x} \begin{pmatrix}
1 \\
0 \\
\frac{c}{\lambda + mc^2} P_z \\
\frac{1}{E + mc^2} (P_x + iP_y)
\end{pmatrix}
\]  

where \( E = \sqrt{m^2 c^4 + P^2 c^2} \) is the relativistic energy-momentum relationship. The wavefunction that satisfies the Dirac equation should be the superposition of eigenstates of Eq.7

\[
\psi(x) = N \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \psi(P) u(P) dP_x dP_y dP_z
\]

\[
\psi(P) = e^{-i\frac{\lambda}{2} P \cdot x} e^{-i\frac{\lambda}{2} P \cdot y} e^{-i\frac{\lambda}{2} P \cdot z} e^{\frac{P^2 c^2}{\lambda} + \frac{P \cdot x + P \cdot y + P \cdot z}{\lambda}}
\]

\[
u(P) = \begin{pmatrix}
1 \\
0 \\
\frac{1}{2mc} P_z \\
\frac{1}{2mc} (P_x + iP_y)
\end{pmatrix}
\]

where we keep the momentum up to the quadratic terms \( P^2 = P_x^2 + P_y^2 + P_z^2 \) for \( P \ll mc \) when \( d \gg \lambda_c \). \( \lambda_c = \hbar/mc = 3.862 \times 10^{-13} \) is the reduced Compton wavelength. We shall not omit the \( \frac{\lambda c}{2mc} \) factors in the spinor because they are responsible for the circulating flow of the current density, nor shall we neglect the momentum-dependent temporal factors \( e^{-i\frac{\lambda}{2} P \cdot x} \) because they are responsible for the decoherence of the electron wavepacket.

Eq.8 is then consolidated into a compact form after performing momentum integral over all directions.

\[
\psi(x) = N e^{-i\frac{\lambda}{2} x^2 / \hbar} G(x, y, z, t) \begin{pmatrix}
1 \\
0 \\
\frac{1}{2mc} d^2 + i\hbar t/m \right) (x + iy)
\end{pmatrix}
\]

\[
\text{where } N \text{ is the normalization factor and } G(x, y, z, t) \text{ represents the time-dependent Gaussian profile}
\]

\[
G(x, y, z, t) = \left( \frac{2\hbar^2 \pi}{d^2 + i\hbar t/m} \right)^{3/2} e^{-\frac{x^2 + y^2 + z^2}{2(d^2 + i\hbar t/m)}}.
\]

Eq.9 is verified to be a solution of the Dirac equation, from which the total charge and current densities are calculated via the definition of Eq.2

\[
\rho(x) = eN^2 G(x, y, z, t)^2 \left[ 1 + \frac{\lambda_c^2 x^2 + y^2 + z^2}{2 d^4 + (\lambda_c c t)^2} \right]
\]

\[
j(x) = ecN^2 G(x, y, z, t)^2 \times \frac{\lambda_c}{d^2 + i\hbar c t} (-y, x, \lambda_c c t d^2 + i\lambda_c c t z).
\]

Eqs.10 recovers the circulating flow for the total current density, where the \( x \) component of \( j \) is a function of \( y \) and vice versa. The above charge and current densities are time-dependent, but at \( t = 0 \) they reduce to the same result as the restricted wavepacket in Ref.7.

As time lapses, Eqs.11 shows that decoherence occurs quickly for both the charge and current densities due to the time-dependent terms \( e^{-i\frac{\lambda c}{2mc} t} \) that are not included in the previous treatment 7. Different eigenstates have different temporal phase factors to cause dephase over time. The decoherence time can be estimated from Eq.11 to be in the order of \( t \approx \lambda_c c / d^2 \), which is about \( 8.638 \times 10^{-13} \)s for a wavepacket size of \( d = 10 \) nm. The short-lived wavepacket suggests a free electron wavepacket may be constructed but can not survive long enough for practical applications.

III. DIRAC ELECTRON INSIDE A TWO-DIMENSIONAL WELL

It is known that stable waves can be produced by confinement. We turn our attention to a simplest confinement: a two-dimensional infinite potential well. With the progress in nano and material technologies, such configuration can be actually fabricated, providing the opportunity for a real case study.

We assume the well to have zero potential inside the region of \( x = -L, L, \) and \( y = -L, L \) and infinite potential outside. We assume there is no confinement in the \( z \)-direction and let \( P_z = 0 \). The correct waveform of the

| Name and symbol | Value | Unit |
|----------------|-------|------|
| Electron charge \( e \) | \(-1.6022 \times 10^{-19} \) | C |
| Electron mass \( m \) | \(9.109 \times 10^{-31} \) | Kg |
| Vacuum permeability \( \mu_0 \) | \(1.257 \times 10^{-6} \) | H/m |
| Speed of light \( c \) | \(2.998 \times 10^8 \) | m/s |
| Reduced Planck constant \( \hbar \) | \(1.054 \times 10^{-34} \) | JHs^{-1} |
lowest energy eigenstate is found

$$\psi(x) = Ne^{-i\Phi E\tau} \cos \frac{\pi x}{2L} \cos \frac{\pi y}{2L}$$

$$\times \left( \begin{array}{ccc} 1 \\ 0 \\ 0 \\ \eta \tan \frac{\pi x}{2L} - \eta \tan \frac{\pi y}{2L} \end{array} \right)$$

(12)

where $\eta = \frac{h}{E + mc^2}$ is a dimensionless geometric factor, which becomes larger for tighter confinement. We study the ground state for this work and leave the excited states for future discussion.

The normalization factor $N = 1 / \left( L \sqrt{1 + 2\eta^2} \right)$ is obtained after invoking the unity equation $\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \psi^* \psi \, dx \, dy = 1$.

The energetic phase factor $e^{-i\Phi E\tau}$ is separated entirely from the spatial wavefunction and the spinor. The separation of variables is verified by plugging Eq.12 into the Dirac equation Eq.1 to obtain the eigenvalue equation:

$$\left[-i \frac{1}{c} \frac{E}{\hbar} + i \frac{mc}{\hbar} + 2i \left( \frac{\pi}{2L} \right)^2 \frac{h}{E + mc^2} \right] \psi(x) = 0$$

(13)

that gives the energy eigenvalue for the ground state,

$$E = \sqrt{m^2 c^4 + 2 \left( \frac{h \pi}{2L} \right)^2}.$$

(14)

Eqs. 12 is the exact ground eigenstate for the Dirac electron in the two-dimensional quantum well, which results in the stable charge density

$$\rho(x) = eN^2 \left( \cos \frac{\pi x}{2L} \cos \frac{\pi y}{2L} \right)^2 \left[ 1 + \eta^2 \left( \tan \frac{\pi x}{2L} + \tan \frac{\pi y}{2L} \right) \right]$$

and stable current density

$$j(x) = ecN^2 \left( \cos \frac{\pi x}{2L} \cos \frac{\pi y}{2L} \right)^2 \eta \left( -\tan \frac{\pi y}{2L}, \tan \frac{\pi x}{2L}, 0 \right).$$

(15)

Next, the vector plot of Eq.16 in Fig.2 confirms the circulating flow pattern. The flow is predominantly circular in the middle but gradually becomes parallel to the wall at the boundaries, showing the influence from the boundaries to the spin.

The total current density distribution of Eq.17 in Fig.3 displays a deep crater large enough to host the charge profile. Figs. 2 and 3 illustrate the picture of the total current circulating around the charge profile at a scale determined by the quantum well, in contrast to the spinning particle picture. Also the undulation on the ridge indicates the interference from the $x$ and $y$ direction waves.

With the help of Eqs. 15,16,17 numerical calculation is carried out to visualize the charge and total current densities. We choose a realistic dimension $L = 10 \text{ nm}$ for the quantum well, which gives a small but appreciable geometric factor $\eta = 3.033 \times 10^{-5}$.

First, the charge distribution in Fig.1 is shown confined in the well. The density peaks at the center and distributes symmetrically within the well as expected.

FIG. 1. The charge density distribution plot for the ground eigenstate of an electron in the quantum well of $L = 10 \text{ nm}$. The $z$ axis represents the charge density of the relative unit.

FIG. 2. The vector plot of the total current density for the ground eigenstate of an electron in the quantum well of $L = 10 \text{ nm}$. 

FIG. 3. The topography for the charge and current density distribution are illustrated in Fig.4. The donut shape of the current density is explained by the product of the charge and velocity in $j = \rho v$, where the velocity $v$ starts at zero at the center but increases radially as expressed...
FIG. 3. 3D plot of the total current density distribution for the ground eigenstate of an electron in the quantum well of $L = 10 \text{ nm}$. The z-axis represents the current density of the relative unit.

FIG. 4. The density plots for the charge (left) and total current density (right) for the ground eigenstate of an electron inside a quantum well of $L = 10 \text{ nm}$.

by $v = j/\rho$

$$v(x) = \frac{2\eta}{c} \sqrt{\frac{\tan^2 \frac{\pi x}{2L} + \tan^2 \frac{\pi y}{2L}}{1 + \eta^2(\tan^2 \frac{\pi x}{2L} + \tan^2 \frac{\pi y}{2L})}},$$  \hspace{0.5cm} (18)$$

which is zero at center and bounded by the speed of light $c$, thus avoids the aforementioned obstacle in the particle spin model.

The same wavefunction of Eq. (12) that produces the circulating total current density yields the electron spin density $s(x)$ and the total electron spin $S$

$$s(x) = \frac{\hbar}{2} \psi^*(x) \sigma \psi(x)$$

$$= \frac{\hbar}{2} N^2 \left( \cos \frac{\pi x}{2L} \cos \frac{\pi y}{2L} \right)^2$$

$$\left(0, 0, 1 - \eta^2 \left(\tan^2 \frac{\pi x}{2L} + \tan^2 \frac{\pi y}{2L}\right)\right),$$  \hspace{0.5cm} (19)$$

$$S = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} s(x) dx dy = \left(0, 0, \frac{\hbar}{2} \left(1 - 2\eta^2 \right)\right).$$  \hspace{0.5cm} (20)$$

where $\sigma$ is the $4 \times 4$ spin operator.

Eq. (20) shows that the electron spin value $\hbar/2$ is modified by the geometric factor $\eta$, as a result of the wave nature of the spin.

IV. DISCUSSION AND CONCLUSION

This work continues the discussion of wave interpretation of the electron spin following Belinfante, Ohanian, and Sebens. In summary,

1. We solve the exact eigenstates of the Dirac equation for an electron inside a two-dimensional quantum well that results in a 4-spinor containing wavefunction and geometry factor.

2. A stable circulating total current density calculated from the above eigenstate demonstrates a donut-shaped distribution. The calculated spin value is modified by the well geometry.

3. We also analyze the free electron Gaussian wavepacket with the superposition of a complete set of time-dependent plane-wave eigenstates. The result shows that the wavepacket is not stable and experiences quick decoherence.

The wave nature of the spin can have critical implications for emerging technologies. The electron spin can potentially be an essential building block for quantum computing \[10\] and quantum information \[11\]. As shown in the paper, isolation of the wave spin from the environment is impossible due to the boundary effects to the wave. In addition, any geometric and material changes to the boundaries can further perturb the spin, which leads to errors in the storing, transmitting, and processing of information.

On the other side, we can use the wave nature of the spin to devise novel schemes for spin readout by probing and even mapping the current or spin densities. Mapping these properties is possible because they are observable quantities that reside entirely outside the particle electron, as shown in Figs. 3 and 4. It is conceivable that the wave spin may open up the path to more holographic and parallel schemes of quantum computing and quantum information technologies.

Finally, the discussion of the wave or particle spin is characterized best by using the 4-spinor such as

$$\begin{pmatrix} 1 \\ 0 \\ 0 \\ \eta \tan \frac{\pi x}{2L} - \eta \tan \frac{\pi y}{2L} \end{pmatrix}$$

in Eq. (12) which contains both the wavefunction and geometry factor, or using the 2-spinor $\begin{pmatrix} 1 \\ 0 \end{pmatrix}$ that appears to depict a dimensionless particle spin.

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