Quantum mechanics of a fermion confined to a curved surface in Foldy-Wouthuysen representation

Hao Zhao,[1,2] Yong-Long Wang,[2,3,*] Cheng-Zhi Ye,[2] Run Cheng,[1,2] Guo-Hua Liang,[4] and Hui Liu[1]

[1]*Department of Physics, Nanjing University, Nanjing 210093, China*
[2]*School of Physics and Electronic Engineering, Linyi University, Linyi 276000, China*
[3]*Laboratory of Solid State Microstructures, Nanjing University, Nanjing 210093, China*
[4]*School of Science, Nanjing University of Posts and Telecommunications, Nanjing 210023, China*

(Received 28 November 2021; revised 20 April 2022; accepted 10 May 2022; published 25 May 2022)

In Foldy-Wouthuysen representation, this paper deduces the effective quantum mechanics for a relativistic particle confined to a curved surface in an external field by using the thin-layer quantization scheme. It is found that the quantum effects caused by introducing the confining potential can be taken as the results of relativistic correction in the nonrelativistic limit. Meanwhile, the spin connection of the curved surface can produce a Zeeman-like gap through the relativistic correction term. In addition, the confining potential can provide a curvature-independent energy shift resulting from the *Zitterbewegung* effect. As an example, this paper applies the effective Hamiltonian to a torus surface, in which the spin effects related to the introduced confining potential are obtained. These results demonstrate the scaling of the noncommutation of the nonrelativistic limit and the thin-layer quantization procedure.

DOI: 10.1103/PhysRevA.105.052220

I. INTRODUCTION

With the rapid development of nanotechnology, more and more nanostructures with complex geometries can be fabricated [1–4]. The presence of geometries enables the nanosystems to have some novel quantum effects. Two important ingredients are the geometric potential [5] and geometric momentum [6,7], both of which are induced by curvature. Subsequently, the curvature-induced effects were extensively investigated in thin magnetic shells [8,9], nematic shells [10], titania single crystals [11], smectic liquid crystals [12], a quantum spin Hall system [13], photonic crystal fibers [14], domain wall pinning [15], domain wall motion [16], antiferromagnets [17], etc. For the particle or quasiparticle confined to a two-dimensional (2D) curved surface, the effective quantum dynamics can be effectively given in the thin-layer quantization formalism [5,18,19]. The validity of the quantization approach was recently proven in experiments. Specifically, the geometric potential was experimentally observed in topological crystal [20], and the geometric momentum was found to affect plasmon polarization [21]. The thin-layer quantization approach is effective, and it has been expanded to the classical field, a particle with spin, etc. Specifically, the thin-layer quantization approach was successfully employed to obtain the effective Maxwell's equation [22–24] describing the electromagnetic wave propagation along a curved surface, the effective Schrödinger equation [25] describing the particle confined to a curved surface, the effective Pauli equation [26–28] describing the nonrelativistic particle with a spin confined to a curved surface, and the effective Dirac equation [29–35] describing the relativistic particle confined to a curved surface.

The thin-layer quantization formalism is valid and successful, but some problems need to be further discussed. One is the noncommutation relationship of the nonrelativistic limit and the thin-layer quantization procedure [36]. For a relativistic fermion in an external field, the nonrelativistic limit can contribute to an additional coupling of magnetic moment and external field, without effective spin-orbit coupling and energy correction induced by the external field. However, in the Foldy-Wouthuysen representation (FWR) [37–41], the two components of positive- and negative-energy states can be decoupled step by step and thus lead to an effective spin-orbit coupling and an effective energy correction in the effective quantum dynamics. In addition, in FWR, the effective quantum mechanics can well illustrate the effects of the field-induced Darwin term [42,43] and the spin precession [44–46] in superconducting materials and valley electronics devices. For a nonrelativistic electron confined to a 2D curved surface, an effective moment induced by geometry [47] will couple with the external field in the thin-layer quantization procedure. Therefore it is interesting to reconsider a relativistic electron confined to a curved surface in FWR.

This paper considers a relativistic electron confined to a curved surface in an external field in FWR and discusses the effective quantum dynamics in the thin-layer quantization formalism. The rest of this paper is organized as follows. In Sec. II, the Dirac equation in a stationary curved space-time and the Foldy-Wouthuysen transformation (FWT) are briefly reviewed. In Sec. III, a relativistic electron confined to a curved surface S in an external field is considered, and the effective Dirac Hamiltonian in FWR is presented by using the thin-layer quantization approach. Interestingly, the effective Hamiltonian contains a coupling of spin connection and

*wangyonglong@lyu.edu.cn

 ©2022 American Physical Society

external field, which can lead to a Zeeman-like effect. As an example, the particular curvature-induced Zeeman splitting is demonstrated on a torus surface. Finally, Sec. IV concludes this paper.

II. DIRAC EQUATION AND ITS FOLDY-WOUTHUYSEN REPRESENTATION

In this section, the Dirac equation in a curved space-time and the FWT in an external field are briefly reviewed. A relativistic electron in a curved space-time can be described by a Dirac equation, that is,

$$(i\gamma^{\mu}\nabla_{\mu} - m)\Phi = 0, \tag{1}$$

where ∇_{μ} is a covariant derivative with $\nabla_{\mu} = \partial_{\mu} + \Gamma_{\mu}$. Γ_{μ} denotes a spin connection, and $\mu = 0, 1, 2, 3$ stands for the four coordinate variables of the curved space-time. γ^{μ} is a Dirac matrix defined in the curved space-time, and it can be expressed as

$$\gamma^{\mu} = E^{\mu}_{\alpha}\gamma^{\alpha},$$

where γ^{α} is an ordinary Dirac matrix defined in a flat space-time. $\alpha = 0, 1, 2, 3$ stands for the four coordinate variables of the flat space-time, and E^{μ}_{α} are vierbeins defined by

$$E^{\mu}_{\alpha} = \frac{\partial q^{\mu}}{\partial x^{\alpha}},$$

where q^{μ} stands for a coordinate variable of the curved space-time and x^{α} stands for a coordinate variable of the flat space-time. With the vierbeins ${E^{\mu}}_{\alpha}$, the inverse of the metric tensor defined in the four-dimensional curved space-time $G^{\mu\nu}$ can be expressed as

$$G^{\mu\nu} = E^{\mu}_{\alpha}E^{\nu}_{\beta}\eta^{\alpha\beta},$$

where $\eta^{\alpha\beta}$ is the inverse metric tensor defined in the four-dimensional flat space-time and $\eta^{\alpha\beta} = \mathrm{diag}(-1, 1, 1, 1)$. Through $\Gamma^{\nu}_{\kappa\mu}$ and $\Sigma_{\alpha\beta}$ the spin connection Γ_{μ} can be described as

$$\Gamma_{\mu} = \tfrac{1}{4}E^{\alpha}_{\nu}\left(\partial_{\mu}E^{\nu\beta} + \Gamma^{\nu}_{\kappa\mu}E^{\kappa\beta}\right)\Sigma_{\alpha\beta},$$

where $\Gamma^{\nu}_{\kappa\mu}$ is the Christoffel symbol and $\Sigma_{\alpha\beta} = [\gamma_{\alpha}, \gamma_{\beta}]/2$. For simplicity and without loss of generality, ds^2 can be described with a stationary space-time as

$$ds^2 = -G_{00}dq^0dq^0 + G_{\mathrm{AB}}dq^Adq^B,$$

where $G_{00} = 1$ and $A, B = 1, 2, 3$ stand for the three coordinate variables of the curved space. Therefore ${E_{\nu}}^{\alpha}$ can be simplified in the following form:

$${E_{\nu}}^{\alpha} = \begin{pmatrix} 1 & 0 \\ 0 & E^{I}_{A} \end{pmatrix},$$

where $I = 1, 2, 3$ stands for the three coordinate variables of the flat space. The space components of Dirac matrices γ^A can be expressed as $\gamma^A = {E^A}_I\gamma^I$. In the stationary space-time, the Dirac Eq. (1) can be simplified in the form of the Schrödinger equation,

$$H\Phi = E\Phi,$$

where H is a Dirac Hamiltonian, that is,

$$H = -i\beta\gamma^A\nabla_A + \beta m,$$

where β is γ^0, a Dirac matrix, and γ^A stands for a reduced Dirac matrix defined in the curved space.

In the relativistic case, the quantum mechanics can be described by a Dirac equation that is a first-order differential equation. In the nonrelativistic limit case, the quantum dynamics is usually described by a Pauli equation that is a second-order differential equation. In view of the differential orders of the quantum dynamical equations, the performing order of the thin-layer quantization scheme is crucial because the second-order derivative operators can exhibit more geometry-induced effects than the first-order ones in the effective quantum dynamics. Ultimately, the nonrelativistic limit and the thin-layer quantization scheme are generally noncommutative. According to the noncommutation, the actions of the nonrelativistic limit on the geometric effects (which are obtained in the thin-layer quantization formalism) need further discussion to be more detail. This paper considers a relativistic particle in the presence of an external electric field and discusses it in FWR.

As an example, this paper considers a relativistic electron in an external field that can be described by a Dirac Hamiltonian,

$$H = -i\beta\gamma^A\nabla_A + \beta m + \beta V, \tag{2}$$

where $\beta = \gamma^0$, $\nabla_A = \partial_A + \Gamma_A + \mathcal{A}_A$. $\mathcal{A}_A$ is a vector potential, and V is a scalar potential. Under the FWT, the Dirac Hamiltonian (2) can be simplified as

$$H = \beta m + \mathcal{E} + \mathcal{O}, \tag{3}$$

where $\mathcal{E} = \beta V$ is an even form that commutes with β and $\mathcal{O} = -i\beta\gamma^A\nabla_A$ is an odd form that anticommutes with β. To decouple the two components of positive and negative energy, the first unitary operator e^{iS} can be expressed by the odd term $\mathcal{O}$ with $S = \frac{-i\beta\mathcal{O}}{2m}$. With the first unitary operator e^{iS}, the Dirac Hamiltonian Eq. (3) can be transformed into

$$H_{\mathrm{FW}} = e^{iS}He^{-iS} = \beta m + \beta\mathcal{E} + \frac{\beta}{2m}\mathcal{O}^2 - \frac{1}{8m^2}[\mathcal{O}, [\mathcal{O}, \mathcal{E}]] + \frac{\beta}{2m}[\mathcal{O}, \mathcal{E}] - \frac{1}{3m^2}\mathcal{O}^3 + \cdots, \tag{4}$$

where H_{FW} is a new Dirac Hamiltonian that is added by two even terms $\frac{\beta}{2m}\mathcal{O}^2$ and $-\frac{1}{8m^2}[\mathcal{O}, [\mathcal{O}, \mathcal{E}]]$, and it is replaced by two new odd terms $\frac{\beta}{2m}[\mathcal{O}, \mathcal{E}]$ and $-\frac{1}{3m^2}\mathcal{O}^3$. To transform the original Dirac Hamiltonian into a block-diagonal form, i.e., eliminate the off-diagonal elements, the second unitary operator can be taken as e^{iS_2} with $S_2 = \frac{-i\beta\mathcal{O}_2}{2m}$ and $\mathcal{O}_2 = \frac{\beta}{2m}[\mathcal{O}, \mathcal{E}]$, and the third unitary operator can be given by e^{iS_3}, with $S_3 = \frac{-i\beta\mathcal{O}_3}{2m}$ and $\mathcal{O}_3 = -\frac{1}{3m^2}\mathcal{O}^3$. It is obvious that the above unitary transformations will converge when the m term is much larger than the others in Eq. (3). Generally, the effective mass of an electron is of the order of mega-electron-volts (MeV), and the rest of the terms are of the order of approximately milli-electron-volts (meV) to electron volts (eV) in ordinary Dirac matter. As an effective approximation, the former four terms in Eq. (4) can be taken as an effective Hamiltonian in FWR.

III. THE EFFECTIVE QUANTUM MECHANICS FOR A RELATIVISTIC ELECTRON CONFINED TO A CURVED SURFACE IN FWR

In this section, the effective quantum mechanics in FWR will be discussed for a relativistic electron confined to a 2D curved surface embedded in a three-dimensional Euclidean space. For convenience, a curvilinear coordinate system spanned by (q_1, q_2, q_3) can be adapted, where q_1 and q_2 are two tangent coordinate variables of S and q_3 is a normal one. Therefore, in a small neighborhood of S denoted as ΞS, the position vector of the point can be parametrized by

$$\vec{R}(q_1, q_2, q_3) = \vec{r}(q_1, q_2) + q_3\vec{n}(q_1, q_2), \tag{5}$$

where $\vec{r}(q_1, q_2)$ denotes the position vector of a point on S and $\vec{n}(q_1, q_2)$ is the normal unit basis of S, which is a function of q_1 and q_2. With Eq. (5), the covariant elements of the metric tensor G_{AB} in ΞS can be defined by

$$G_{AB} = \frac{\partial\vec{R}}{\partial q^A}\cdot\frac{\partial\vec{R}}{\partial q^B}.$$

The covariant elements of the metric tensor g_{AB} defined on S can be defined by

$$g_{ab} = \frac{\partial\vec{r}}{\partial q^a}\cdot\frac{\partial\vec{r}}{\partial q^b},$$

where $a, b = 1, 2$ stand for the two tangent coordinate variables of S. In terms of the two definitions of G_{AB} and g_{ab}, it is easy to prove that the covariant elements G_{ab} and g_{ab} satisfy the following equation:

$$G_{ab} = g_{ab} + q_3[\alpha g + (\alpha g)^T]_{ab} + q_3^2(\alpha g\alpha^T)_{ab}, \tag{6}$$

$G_{a3} = G_{3a} = 0, G_{33} = 1$, where α is the Weingarten curvature tensor described by

$$\alpha_{ab} = \frac{\partial\vec{r}}{\partial q^a}\cdot\frac{\partial\vec{n}}{\partial q^b}.$$

In ΞS and with the adapted coordinate system of (q_1, q_2, q_3), the vierbeins E_A^I can be expressed as

$$E_A^I = \begin{pmatrix} E_a^i & 0\\ 0 & 1\end{pmatrix}, \tag{7}$$

where

$$\begin{aligned} E_a^i &= e_a^i + q_3\alpha_a^b e_b^i,\\ E_i^a &= e_i^a - q_3\alpha^a{}_b e^b{}_i + O\big[q_3^2\big]. \end{aligned} \tag{8}$$

With the vierbeins and their inverses, the reduced Dirac matrices γ^a can be described by $\gamma^a = E_i^a\gamma^i$, and γ^3 is invariant.

A. The effective Hamiltonian on a curved surface in FWR

According to the thin-layer quantization scheme, this paper introduces a confining potential $V(q_3)$ to confine the relativistic electron to S. For simplicity and without loss of generality [48], the electron is confined to S by a square-well potential type. It is zero on the surface and goes to infinity elsewhere. Subsequently, the Dirac Hamiltonian should be replaced by

$$H = -i\beta\gamma^A\nabla_A + \beta m + \beta V(q_3), \tag{9}$$

where $V(q_3)$ is the introduced confining potential and $\nabla_A = \partial_A + \Gamma_A$. Obviously, the term $-i\beta\gamma^A\nabla_A$ is odd. Therefore the first unitary operator for FWT can be given by $U_1 = e^{iS_1}$, and $S_1 = \frac{-\gamma^A\nabla_A}{2m}$. The first transformed Hamiltonian can be obtained as

$$\begin{aligned} H_{\rm FW} &= e^{iS_1}He^{-iS_1}\\ &= \beta m + \beta V(q_3) + \frac{\beta}{2m}(\gamma^A\nabla_A)^2\\ &\quad + \frac{1}{8m^2}[\beta\gamma^A\nabla_A, [\beta\gamma^A\nabla_A, \beta V(q_3)]]\\ &\quad + \frac{-i\beta}{2m}[\beta\gamma^A\nabla_A, \beta V(q_3)] - \frac{i}{3m^2}(\beta\gamma^A\nabla_A)^3 + \cdots. \end{aligned} \tag{10}$$

On the right-hand side, the first four terms are even, and the last two terms are odd. In order to diagonalize the two odd terms, we need to introduce the second unitary operator $U_2 = e^{iS_2}$ and the third unitary operator $U_3 = e^{iS_3}$, where $S_2 = \frac{-1}{4m^2}[\beta\gamma^A\nabla_A, \beta V(q_3)]$ and $S_3 = \frac{-\beta}{6m^3}(\beta\gamma^A\nabla_A)^3$. With e^{iS_2} and e^{iS_3}, the first transformed Hamiltonian can be transformed into

$$\begin{aligned} H_{\rm FW}^1 &= e^{iS_3}e^{iS_2}H_{\rm FW}e^{-iS_2}e^{-iS_3}\\ &= e^{iS_3}e^{iS_2}e^{iS_1}He^{-iS_1}e^{-iS_2}e^{iS_3}\\ &= \beta m + \beta V(q_3) + \frac{\beta}{2m}(\gamma^A\nabla_A)^2\\ &\quad + \frac{1}{8m^2}[\beta\gamma^A\nabla_A, [\beta\gamma^A\nabla_A, \beta V(q_3)]] + \cdots. \end{aligned} \tag{11}$$

It is straightforward that $H_{\rm FW}^1$ is a power series of $\frac{1}{m}$. When the energy contributed by the effective mass m plays a dominant role in Eq. (11), $H_{\rm FW}^1$ converges. Generally, in a Dirac material the effective mass of the electron corresponds to MeV, the confining potential corresponds to eV, and the momentum corresponds to meV. As a consequence, the effective Hamiltonian is limited to the first four terms and denoted as $H_{\rm EFW}$.

In the squeezing process of the thin-layer quantization formalism, the differential homeomorphism transformation induced by the presence of curvature should be considered. Specifically, the curvature-induced transformation can be described by the relationship $G = f^2g$, where G is the determinant of G_{AB} defined in ΞS, g is the determinant of g_{ab} defined on S, and f is the rescaling factor with $f = 1 + Tr(\alpha)q_3 + \det(\alpha)q_3^2$. Under the rescaling transformation, the wave function Φ and the Dirac Hamiltonian $H_{\rm FW}$ satisfy the following transformations:

$$\begin{aligned} \psi &= f^{1/2}\Phi,\\ \bar{H}_{\rm FW} &\to f^{\frac{1}{2}}H_{\rm FW}f^{-\frac{1}{2}}, \end{aligned} \tag{12}$$

where ψ and $\bar{H}_{\rm FW}$ are a new wave function and a new Dirac Hamiltonian, respectively. By expanding the Hamiltonian $\bar{H}_{\rm FWT}$ as a power series of q_3 and limiting $q_3 = 0$, the effective Dirac Hamiltonian confined to S can be obtained as

$$\bar{H}_{\rm EFW} = \beta m + \beta V(q_3) + H'_{\rm FW} + H''_{\rm FW}, \tag{13}$$

where

$$H'_{\rm FW} = \frac{\beta}{2m}\Bigg\{[\bar{\gamma}^a(\partial_a + \Omega_a)][\bar{\gamma}^b(\partial_b + \Omega_b)] + \partial_3^2 - \gamma^3\alpha^a{}_b e^b{}_i\gamma^i\partial_a + \gamma^3\alpha^a{}_b e^b{}_i\gamma^i\left(\Omega_a + \frac{1}{2}\epsilon^a_b\bar{\gamma}_a\gamma^3\alpha^a_a\right) + \gamma^3\bar{\gamma}^a\partial_3\Gamma_a + \partial_3\Gamma_3 + |\epsilon^a_b|\alpha^a{}_b\alpha^b{}_a/2\Bigg\}, \tag{14}$$

where in $\bar{\gamma}^a = e^a_i\gamma^i$ is the reduced Dirac matrix defined on S, Ω_a is the normal part of the spin connection Γ_a that does not depend on q_3, and ϵ is a second-order matrix whose antidiagonal elements are 1 and whose other elements are zero. In Eq. (13), the last term, $H''_{\rm FW}$, is

$$H''_{\rm FW} = -\frac{V(q_3)}{m}H'_{\rm FW} - \frac{\beta}{8m^2}\big[2\gamma^3(\partial_3 V(q_3))\bar{\gamma}^a(\partial_a + \Omega_a) + 4(\partial_3 V(q_3))\partial_3 + \big(\partial_3^2 V(q_3)\big)\big]. \tag{15}$$

Obviously, $H'_{\rm FW}$ results from the term $\frac{\beta}{2m}(\gamma^A\nabla_A)^2$, and $H''_{\rm FW}$ results from the term $\frac{1}{8m^2}[\beta\gamma^A\nabla_A, [\beta\gamma^A\nabla_A, \beta V(q_3)]]$ in $\bar{H}_{\rm EFW}$. $H'_{\rm FW}$ and $H''_{\rm FW}$ are proportional to β, and they are block diagonal. Also, the two blocks are opposite to each other.

The thin-layer quantization scheme aims to separate the surface component from the normal one in $\bar{H}_{\rm EFW}$ analytically. Analytically, the terms $\beta m + \beta V(q_3) + H'_{\rm FW}$ can be divided into a normal component,

$$H_n = \beta V(q_3) + \beta\partial_3^2, \tag{16}$$

and a surface component,

$$H_s = \beta m + \frac{\beta}{2m}\Bigg\{[\bar{\gamma}^a(\partial_a + \Omega_a)][\bar{\gamma}^b(\partial_b + \Omega_b)] - \gamma^3\alpha^a{}_b e^b_i\gamma^i\partial_a + \gamma^3\alpha^a_b e^b_i\gamma^i\left(\Omega_a + \frac{1}{2}\epsilon^a_b\bar{\gamma}_a\gamma^3\alpha^a_a\right) + \gamma^3\bar{\gamma}^a\partial_3\Gamma_a + \partial_3\Gamma_3 + |\epsilon^a_b|\alpha^a_b\alpha^b_a/2\Bigg\}. \tag{17}$$

The effective surface Hamiltonian H_s consists of two diagonal blocks, i.e., positive- and negative-energy components. In H_s, Ω_a plays the role of a pseudomagnetic field that is induced by Gauss curvature [30], the term $-\gamma^3\alpha^a_b e^b_i\gamma^i\partial_a$ stands for a spin-orbit coupling that agrees well with the result given in Ref. [30], and the terms $\gamma^3\alpha^a_b e^b_i\gamma^i(\Omega_a + \frac{1}{2}\epsilon^a_b\bar{\gamma}_a\gamma^3\alpha^a_a) + \gamma^3\bar{\gamma}^a\partial_3\Gamma_a$ play the role of Zeeman-like splitting, which is contributed by the gradient of vierbein fields and the normal spin connection. The last term, $|\epsilon^a_b|\alpha^a_b\alpha^b_a/2$, is the known geometric potential [5] resulting from the antidiagonal elements of the Weingarten matrix, and it generally depends on the mean curvature and Gaussian curvature.

In terms of the coupling of the q_3 dependence of the confining potential $V(q_3)$ and the tangent components of the momentum, the term $H''_{\rm FW}$ cannot be analytically separated into surface and normal parts. In comparison with the terms $\beta m + \beta V(q_3) + H'_{\rm FW}$, $H''_{\rm FW}$ is very small to be taken as a perturbation term.

B. The actions of the confining potential

Compared with the effective Pauli equation, the effective Dirac equation contains additional high-power terms of $\frac{1}{m}$ for a relativistic electron confined to S. That is, $H''_{\rm FW}$ is a function of $\frac{1}{m^2}$ that is a relativistic effect added by the presence of the external field. In the external field a moving electron will feel a force, and the coupling of the momentum and spin in the Dirac equation will be modified by the external field. As a consequence, the deformed coupling can provide a spin precession for the moving electron.

In Eq. (9), the mass and $V(q_3)$ are regarded on the same footing for the relativistic mass-energy equivalence via c. In the nonrelativistic limit, the confining potential $V(q_3)$ provides a mass correction proportional to $\frac{V(q_3)}{m}$. Moreover, the normal gradient $\partial_3 V$ can provide an additional force to the relativistic electron by deforming the spin-orbit coupling (SOC). Specifically, the curvature couples with the spin to deform the SOC. The deformation can induce a Zeeman-like splitting. Meanwhile, $\partial_3^2 V(q_3)$ can fluctuate at the normal position of the electron as *Zitterbewegung*, which is caused by the interference between positive- and negative-energy components. As a result, the *Zitterbewegung* can lead to a constant energy shift.

To specifically study the actions of the confining potential on the effective Dirac dynamics, this paper considers three simple examples: (a) $V(q_3) = m\omega|q_3|$, (b) $V(q_3) = m\omega q_3^2$ with ω being a constant, and (c) a deep square well with a small width of L. In case (a), $\partial_3 V(q_3)$ depends on having an m and ω that can be taken as a constant to induce a spin precession correction and Zeeman-like splitting, without *Zitterbewegung* for $\partial_3^2 V(q_3) = 0$. By introducing the confining potential $V(q_3) = m\omega|q_3|$ and by vanishing the terms of q_3, the normal component of Hamiltonian can be given as

$$H_n = \beta V(q_3) + \beta\partial_3^2 - \frac{\beta}{2m}\omega\partial_3 \tag{18}$$

and the effective Dirac Hamiltonian can be obtained as

$$H_{\rm eff} = H_s - \frac{\beta}{4m}\gamma^3\omega\bar{\gamma}^a(\partial_a + \Omega_a). \tag{19}$$

In case (b), $\partial_3 V(q_3) = 2m\omega q_3$ is still a function of q_3 that cannot significantly affect the spin precession and Zeeman-like splitting. $\partial_3^2 V(q_3) = 2m\omega$ just depends on having an m and ω that can be taken as a constant to provide a *Zitterbewegung* effect. Therefore the effective Dirac Hamiltonian should be replaced by

$$H_{\rm eff} = H_s - \frac{\beta}{4m}\omega. \tag{20}$$

In case (c), $H''_{\rm FW}$ directly vanishes on S, and thus the confining potential does not affect the effective Dirac Hamiltonian.

The above discussions indicate that the results are different from the known conclusion given by da Costa [5], i.e., the details of the confining potential do not affect the effective quantum dynamics on a curved surface. Strikingly, the form of the confining potential plays an important role in the effective Dirac Hamiltonian in FWR. Based on this, the effects of the details of the confining potential can be employed to measure the scaling of noncommutation of the nonrelativistic limit and the thin-layer quantization procedure.

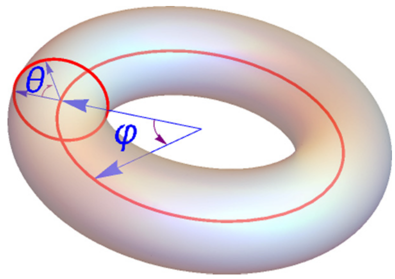

FIG. 1. A torus surface with curvilinear coordinate variables θ and φ.

C. An example: A torus surface

In this section, the previous discussions will be applied to a nanoscale torus that can be parametrized by (θ, φ), shown in Fig. 1. The effective Dirac Hamiltonian in Eq. (17) can be specifically given by

$$H_s = \beta m + \frac{\beta}{2m}\Bigg\{\Big[\bar{\gamma}^{\theta}\partial_\theta + \bar{\gamma}^{\varphi}\Big(\partial_\varphi + i\frac{\sin\theta}{2}\Sigma_3\Big)\Big]^2 - \gamma^3\Big(\frac{1}{r}\bar{\gamma}^{\theta}\partial_\theta + \frac{\cos\theta}{(R + r\cos\theta)}\bar{\gamma}^{\varphi}\partial_\varphi\Big) - i\frac{\cos\theta}{(R + r\cos\theta)}\frac{\sin\theta}{2}\Sigma^{\varphi}\Bigg\}, \tag{21}$$

where Σ^{φ} is a φ Dirac matrix, and the contribution given by the confining potential is

$$H''_{\rm FW} = -\frac{V(q_3)}{m}H'_{\rm FW} - \frac{\beta}{8m^2}\Bigg\{2\gamma^3(\partial_3 V(q_3))\Big[\bar{\gamma}^{\theta}\partial_\theta + \bar{\gamma}^{\varphi}\Big(\partial_\varphi + i\frac{\sin\theta}{2}\Sigma_3\Big)\Big] + 4(\partial_3 V(q_3))\partial_3 + (\partial_3^2 V(q_3))\Bigg\}, \tag{22}$$

where $\bar{\gamma}^{\theta} = e^{\theta}{}_i\gamma^i$ and $\bar{\gamma}^{\theta} = e^{\varphi}{}_i\gamma^i$ are tangent Dirac matrices and $\Sigma_3 = i\gamma_1\gamma_2$ is a normal Dirac matrix.

On the torus surface, the spin connection contained in ∇_θ vanishes, and that in ∇_φ is $\frac{i\sin\theta\Sigma_3}{2}$. The nonvanishing term plays the role of a pseudomagnetic field that produces the Zeeman-like gap. Meanwhile, in $H''_{\rm FW}$, the couplings of curvature can enlarge the Zeeman-like gap. For $\frac{\sin\theta}{2}$, the relevant spin connection and Zeeman-like gap will vanish at $\theta = 0$ or π. For $\frac{\cos\theta}{(R+r\cos\theta)}$, the relevant spin connection and Zeeman-like gap will vanish at $\theta = \frac{\pi}{2}$ or $\frac{3\pi}{2}$. As shown in Fig. 2 , there are opposite Zeeman-like gaps for the spin in the direction φ in the red area and the green area, This is because the Zeeman-like splitting is induced by the Gaussian curvature and its gradient. It is easy to prove that the Gaussian curvature has its maximum value and its gradient vanishes at $\theta = 0$ and π, and the Gaussian curvature vanishes at $\theta = \frac{\pi}{2}$ and $\frac{3\pi}{2}$.

In the spin-orbit interaction terms of H_s, the coefficients are functions of curvature. As a potential application, the Zeeman-like splitting can be manipulated by designing the geometry of the curved surface.

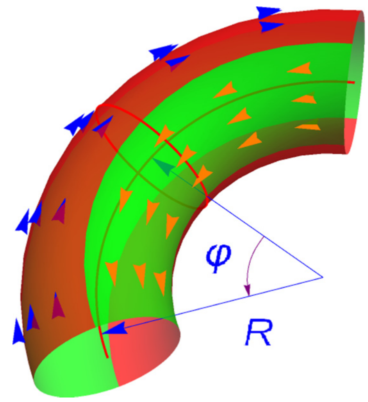

FIG. 2. The different Zeeman-like gaps induced by the Gaussian curvature and its gradient on a torus. There are different directions of gaps in the red area and green area, respectively. The arrowheads denote the directions of splitting.

IV. CONCLUSION

In this paper, the Dirac equation describing a relativistic particle in a stationary curved space-time and the Foldy-Wouthuysen transformation in the presence of an external field are briefly reviewed. In FWR, for the relativistic particle confined to a curved surface in the presence of an external field, the effective Dirac Hamiltonian is deduced by using the thin-layer quantization method. Some interesting terms are induced by the geometry of the curved surface, such as the coupling of spin connections and spin, and that of spin connections and the external field. Those couplings can lead to Zeeman-like splittings. Strikingly, there are two terms (first- and second-order derivatives of q_3) given by the confining potential, which are present in the effective Dirac Hamiltonian. As a result of FWT, the first-order term can lead to a spin precession and a Zeeman-like splitting, while the second-order term can provide a *Zitterbewegung* effect. The results indicate that the noncommutation of the nonrelativistic limit and the thin-layer quantization procedure can be measured.

As an example, the effective Dirac Hamiltonian is given to describe the relativistic electron confined to the torus surface. As expected, the spin connection in the effective Hamiltonian plays the role of a pseudomagnetic field, and it couples with the spin as SOC. The geometry-induced SOC can provide a Zeeman-like gap. These results can be observed in 2D curved graphene materials; the energy gap is widened to several hundred meV at their Dirac points by doping [49,50] or adsorption [51]. On curved hexagonal boron nitride the energy gap is broadened to about 6 eV [52]. These results indicate that the particular properties of spintronic devices and valley electronics can be manipulated by designing their geometries.

ACKNOWLEDGMENTS

This work is jointly supported by the Natural Science Foundation of Shandong Province of China (Grant No. ZR2020MA091), the National Natural Science Foundation of Jiangsu Province of China (Grant No. BK20210581), the National Major State Basic Research and Development of China (Grant No. 2016YFE0129300), the Nanjing

University of Posts and Telecommunications Science Foundation (Grant No. NY221024), the National Natural Science Foundation of China (Grants No. 11690030, No. 11690033, No. 11535005, No. 61425018, and No. 12104239), and the Postgraduate Research & Practice Innovation Program of Jiangsu Province.

[1] T. W. Ebbesen and P. M. Ajayan, Nature (London) **358**, 220 (1992).
[2] N. G. Chopra, R. J. Luyken, K. Cherrey, V. H. Crespi, M. L. Cohen, S. G. Louie, and A. Zettl, Science **269**, 966 (1995).
[3] D. V. Kosynkin, A. L. Higginbotham, A. Sinitskii, J. R. Lomeda, A. Dimiev, B. K. Price, and J. M. Tour, Nature (London) **458**, 872 (2009).
[4] L. Jiao, L. Zhang, X. Wang, G. Diankov, and H. Dai, Nature (London) **458**, 877 (2009).
[5] R. C. T. da Costa, Phys. Rev. A **23**, 1982 (1981).
[6] Q. H. Liu, L. H. Tang, and D. M. Xun, Phys. Rev. A **84**, 042101 (2011).
[7] Y.-L. Wang, H. Jiang, and H.-S. Zong, Phys. Rev. A **96**, 022116 (2017).
[8] Y. Gaididei, V. P. Kravchuk, and D. D. Sheka, Phys. Rev. Lett. **112**, 257203 (2014).
[9] G. Meng, J. Paulose, D. R. Nelson, and V. N. Manoharan, Science **343**, 634 (2014).
[10] G. Napoli and L. Vergori, Phys. Rev. Lett. **108**, 207803 (2012).
[11] S. Yang, B. X. Yang, L. Wu, Y. H. Li, P. Liu, H. Zhao, Y. Y. Yu, X. Q. Gong, and H. G. Yang, Nat. Commun. **5**, 5355 (2014).
[12] D. S. Kim, Y. J. Cha, M. H. Kim, O. D. Lavrentovich, and D. K. Yoon, Nat. Commun. **7**, 10236 (2016).
[13] B. Huang, K.-H. Jin, B. Cui, F. Zhai, J. Mei, and F. Liu, Nat. Commun. **8**, 15850 (2017).
[14] R. Beravat, G. K. L. Wong, M. H. Frosz, X. M. Xi, and P. S. Russell, Sci. Adv. **2**, e1601421 (2016).
[15] K. V. Yershov, V. P. Kravchuk, D. D. Sheka, and Y. Gaididei, Phys. Rev. B **92**, 104412 (2015).
[16] K. V. Yershov, V. P. Kravchuk, D. D. Sheka, and Y. Gaididei, Phys. Rev. B **93**, 094418 (2016).
[17] O. V. Pylypovskyi, D. Y. Kononenko, K. V. Yershov, U. K. Rößler, A. V. Tomilo, J. Fassbender, J. van den Brink, D. Makarov, and D. D. Sheka, Nano Lett. **20**, 8157 (2020).
[18] H. Jensen and H. Koppe, Ann. Phys. (Amsterdam) **63**, 586 (1971).
[19] Y.-L. Wang and H.-S. Zong, Ann. Phys. (Amsterdam) **364**, 68 (2016).
[20] A. Szameit, F. Dreisow, M. Heinrich, R. Keil, S. Nolte, A. Tünnermann, and S. Longhi, Phys. Rev. Lett. **104**, 150403 (2010).
[21] R. Spittel, P. Uebel, H. Bartelt, and M. A. Schmidt, Opt. Express **23**, 12174 (2015).
[22] S. Batz and U. Peschel, Phys. Rev. A **78**, 043821 (2008).
[23] M.-Y. Lai, Y.-L. Wang, G.-H. Liang, F. Wang, and H.-S. Zong, Phys. Rev. A **97**, 033843 (2018).
[24] M.-Y. Lai, Y.-L. Wang, G.-H. Liang, and H.-S. Zong, Phys. Rev. A **100**, 033825 (2019).
[25] G. Ferrari and G. Cuoghi, Phys. Rev. Lett. **100**, 230403 (2008).
[26] T. Kosugi, J. Phys. Soc. Jpn. **80**, 073602 (2011).
[27] M. S. Shikakhwa and N. Chair, Phys. Lett. A **380**, 2876 (2016).
[28] Y.-L. Wang, L. Du, C.-T. Xu, X.-J. Liu, and H.-S. Zong, Phys. Rev. A **90**, 042117 (2014).
[29] F. T. Brandt and J. A. Sánchez-Monroy, Phys. Lett. A **380**, 3036 (2016).
[30] G.-H. Liang, Y.-L. Wang, M.-Y. Lai, H. Liu, H.-S. Zong, and S.-N. Zhu, Phys. Rev. A **98**, 062112 (2018).
[31] G.-H. Liang, Y.-L. Wang, M.-Y. Lai, H. Zhao, H.-S. Zong, and H. Liu, Phys. Rev. A **101**, 053632 (2020).
[32] P. Maraner and J. K. Pachos, Ann. Phys. (Amsterdam) **323**, 2044 (2008).
[33] P. Ouyang, V. Mohta, and R. L. Jaffe, Ann. Phys. (Amsterdam) **275**, 297 (1999).
[34] M. A. Olpak, Mod. Phys. Lett. A **27**, 1250016 (2012).
[35] M. Burgess and B. Jensen, Phys. Rev. A **48**, 1861 (1993).
[36] Y.-L. Wang, H. Zhao, H. Jiang, H. Liu, and Y.-F. Chen, arXiv:2109.09122 [quant-ph].
[37] A. J. Silenko, J. Math. Phys. (Melville, NY) **44**, 2952 (2003).
[38] V. P. Neznamov and A. J. Silenko, J. Math. Phys. (Melville, NY) **50**, 122302 (2009).
[39] L. L. Foldy and S. A. Wouthuysen, Phys. Rev. **78**, 29 (1950).
[40] E. Eriksen, Phys. Rev. **111**, 1011 (1958).
[41] A. J. Silenko, Phys. Rev. A **77**, 012116 (2008).
[42] K. Capelle and E. K. U. Gross, Phys. Rev. B **59**, 7155 (1999).
[43] K. Capelle, Phys. Rev. B **63**, 052503 (2001).
[44] G. Y. Wu, N.-Y. Lue, and L. Chang, Phys. Rev. B **84**, 195463 (2011).
[45] M.-K. Lee, N.-Y. Lue, C.-K. Wen, and G. Y. Wu, Phys. Rev. B **86**, 165411 (2012).
[46] G. Y. Wu and N.-Y. Lue, Phys. Rev. B **86**, 045456 (2012).
[47] F. T. Brandt and J. A. Sánchez-Monroy, Europhys. Lett. **111**, 67004 (2015).
[48] M. Encinosa, L. Mott, and B. Etemadi, Phys. Scr. **72**, 13 (2005).
[49] F. Joucken, L. Henrard, and J. Lagoute, Phys. Rev. Materials **3**, 110301 (2019).
[50] S. Mukherjee and T. Kaloni, J. Nanopart. Res. **14**, 1059 (2012).
[51] M. Papagno, S. Rusponi, P. M. Sheverdyaeva, S. Vlaic, M. Etzkorn, D. Pacilé, P. Moras, C. Carbone, and H. Brune, ACS Nano **6**, 199 (2012).
[52] K. Watanabe, T. Taniguchi, and H. Kanda, Nat. Mater. **3**, 404 (2004).