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Schrödinger Equation of a Particle on a Rotating Curved Surface *

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We derive the Schrödinger equation of a particle constrained to move on a rotating curved surface S. Using the thin-layer quantization scheme to confine the particle on S, and with a proper choice of gauge transformation for the wave function, we obtain the well-known geometric potential $V_{\rm g}$ and an additive Coriolis-induced geometric potential in the co-rotational curvilinear coordinates. This novel effective potential, which is included in the surface Schrödinger equation and is coupled with the mean curvature of S, contains an imaginary part in the general case which gives rise to a non-Hermitian surface Hamiltonian. We find that the non-Hermitian term vanishes when S is a minimal surface or a revolution surface which is axially symmetric around the rolling axis.

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The advent and development in synthesizing low-dimensional nanostructures with curved geometries[1−3] has reignited the interest in the quantum physics on a curved two-dimensional (2D) surface for theoretical physicists. Particles constrained to move in the 2D nanostructures with characteristic dimensions less than the mean free path are ballistic and are described by the quasi-two-dimensional Schrödinger equation.[4,5] Historically, two relevant theoretical approaches have been proposed to describe the quantum behaviors of the particles on a 2D curved surface: a method by DeWitt[6] that deals with the problem by studying the quantum dynamics as fully 2D with constraint, and the other by Jensen *et al.*,[7] and da Costa[8] (JKC) that considers the quasi-2D quantum motion as the squeezing procedure of the motion in a three-dimensional (3D) space subjected to a strong confining potential acting perpendicular to the surface.[9,10] By contrast, the JKC approach has gained a broad consensus in low-dimensional physics since it is well-defined and has been testified by the experimental realization of an optical analog of the curvature-induced quantum geometric potential (QGP).[11] At the same time, according to the method given by DeWitt, Dirac canonical quantization formalism was enhanced to quantize the motion of a particle constrained on a 2D curved surface.[12−14] For decades, many intriguing physics effects caused by the QGP at the nano-scale have been investigated.[15−22] Moreover, the JKC thin-layer method has been shown to be available in the presence of electromagnetic field[10,23] and spin-orbit interaction,[24,25] and employed to predict spin connection geometric potential in the Pauli equation.[26]

Recently, nano rotator fabrication technology enabled us to produce and manipulate high speed nano rotors which are mostly composed by curved 2D nano structures.[27,28] With the rapid development of nano-scale electromechanics, it is inevitable to extend the JKC quantization scheme to describe the quantum dynamics of particles constrained on a rotating surface. However, to our knowledge, very few studies discussed this problem or provided a universal conclusion. In this Letter, we introduce the Coriolis effect to describe the quantum particles in a rotary reference, and study the quantum dynamics of confined particles moving on a rotating 2D curved surface. This work starts with the derivation of the Schrödinger equation of a spin-less particle confined to move in the neighborhood around a rotating curved surface S in the 3D co-rotational Cartesian coordinates. The equivalent Hamiltonian in such non-inertial frame has an additive Coriolis term. We then give the Schrödinger equation in the co-rotational curvilinear coordinates which have been defined and used by da Costa, and completely decouple the Schrödinger equation into a normal component and a surface component with a proper choice of gauge transformation of the wave function. The geometric potential and the additive Coriolis-induced geometric potential are obtained. Finally, we discuss the loss of Hermiticity caused by the Coriolis effect and two special cases in which the non-Hermitian term vanishes.

In the usual way, an inertial three-dimensional (3D) Euclidean space X is described by three immobile basis vectors $\boldsymbol{e}_1$, $\boldsymbol{e}_2$ and $\boldsymbol{e}_3$, which are perpendicu-

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lar to each other. Time-spatial coordinates for an arbitrary point $\boldsymbol{P}$ in X can be marked as (τ, r^1, r^2, r^3). Let us consider a 2D curved surface rotating around axis $\boldsymbol{e}_3$ with angular velocity ω (Fig. 1). The Schrödinger equation of a spin-less particle, with effective mass m, moving in the immediate neighborhood of the surface S embedded in X is

$$i\hbar\frac{\partial}{\partial\tau}\psi(\tau,\boldsymbol{r}) = \frac{-\hbar^2}{2m}\nabla^2_{\boldsymbol{r}}\psi(\tau,\boldsymbol{r}) + [v_\lambda(\tau,\boldsymbol{r}) + v_{\rm s}(\tau,\boldsymbol{r})]\psi(\tau,\boldsymbol{r}), \quad (1)$$

where $\boldsymbol{r}$ is the position vector in X, $\nabla_{\boldsymbol{r}}$ indicates the spatial gradient in X, v_λ represents the confining potential which is assumed to localize the particle on S, λ is a parameter measuring the strength of the confinement, and $v_{\rm s}$ is the surface potential background. In the general case, both v_λ and $v_{\rm s}$ are functionally dependent on the time-spatial coordinates in X due to the rotation of S.

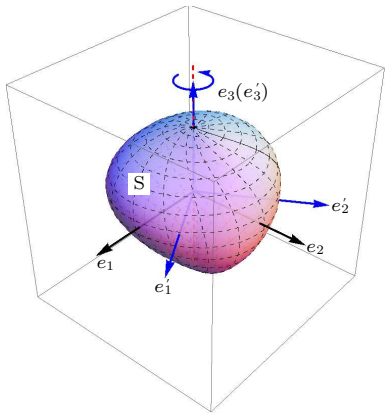

Fig. 1. (Color online) The sketch of an arbitrary surface that rotates around vector $\boldsymbol{e}_3$ ($\boldsymbol{e}_3'$) with angular speed ω.

It is convenient to describe the quantum dynamics of the particles in a co-rotational reference attached to S. We introduce the other reference X' which is composed by three mutual perpendicular basis vectors $\boldsymbol{e}_1'$, $\boldsymbol{e}_2'$ and $\boldsymbol{e}_3'$, and is co-rotating with S. Here X' completely coincides with X at $\tau = 0$ with keeping $\boldsymbol{e}_3'$ overlapping with $\boldsymbol{e}_3$ all the time. In X', the time-spatial coordinates and the wave function are defined as (t, x^1, x^2, x^3) and $\Psi(t,\boldsymbol{x}) = \psi(\tau, \Lambda^{-1}\boldsymbol{x})$ with Λ being the spatial transformation operator which satisfies $\boldsymbol{x} = \Lambda\boldsymbol{r}$, respectively. Moreover, both $v_\lambda(\tau,\boldsymbol{r})$ and $v_{\rm s}(\tau,\boldsymbol{r})$ in Eq. (1) are rewritten as $V_\lambda(\boldsymbol{x}(\tau))$ and $V_{\rm s}(\boldsymbol{x}(\tau))$, respectively, and are not directly functionally dependent on τ. The time and the time derivative transformations from X to X' read (see the content at the end)

$$\tau = t, \quad \frac{\partial}{\partial\tau} = \frac{\partial}{\partial t} - \frac{i}{\hbar}\omega\hat{L}_3, \quad (2)$$

where $\hat{L}_3 = i\hbar(x^1\frac{\partial}{\partial x^2} - x^2\frac{\partial}{\partial x^1})$ is the angular momentum operator along $\boldsymbol{e}_3'$. The transformation for spatial gradient operator from X to X' reads

$$\nabla_{\boldsymbol{r}} = \nabla_{\boldsymbol{x}}, \quad (3)$$

with $\nabla_{\boldsymbol{x}}$ being the spatial gradient in X'. From Eqs. (2) and (3), the Schrödinger equation in X' is

$$i\hbar\frac{\partial}{\partial t}\Psi(t,\boldsymbol{x}) = \Big[\frac{-\hbar^2}{2m}\nabla^2_{\boldsymbol{x}} - \omega\hat{L}_3 + V_\lambda(\boldsymbol{x}) + V_{\rm s}(\boldsymbol{x})\Big]\Psi(t,\boldsymbol{x}), \quad (4)$$

where the Coriolis term $\omega\hat{L}_3$ can be generalized to $\boldsymbol{\omega}\cdot\hat{\boldsymbol{L}}$, with $\boldsymbol{\omega}$ and $\hat{\boldsymbol{L}}$ being the total angular speed vector and the total angular momentum, respectively, and can be rewritten as

$$\boldsymbol{\omega}\cdot\hat{\boldsymbol{L}} = -i\hbar\boldsymbol{\Omega}\cdot\nabla_{\boldsymbol{x}}, \quad (5)$$

with $\boldsymbol{\Omega} = \boldsymbol{\omega}\times\boldsymbol{x}$. Hereafter, we call $\boldsymbol{\Omega}$ the Coriolis factor. The effective Schrödinger equation with time-independent potentials $V_{\rm s}$ and V_λ in the co-rational reference X' reads

$$i\hbar\frac{\partial}{\partial t}\Psi(t,\boldsymbol{x}) = \Big[\frac{-\hbar^2}{2m}\nabla^2_{\boldsymbol{x}} + i\hbar\boldsymbol{\Omega}\cdot\nabla_{\boldsymbol{x}} + V_\lambda(\boldsymbol{x}) + V_{\rm s}(\boldsymbol{x})\Big]\Psi(t,\boldsymbol{x}). \quad (6)$$

We then follow the da Costa-like quantization procedure to derive the separated Schrödinger equation of particles confined on the surface with the Coriolis effect in X'. For the sake of clarity, we start the derivation from illustrating the curvilinear coordinates in X' which is analogous to the one given in Ref. [8]. The surface S can be parameterized as $\boldsymbol{s} = \boldsymbol{s}(q^1, q^2)$ with q^1 and q^2 being the co-rotational curvilinear coordinates over S. The portion of the immediate neighborhood of S, embedded in 3D space, can be described as

$$\boldsymbol{x}(q^1,q^2,q^3) = \boldsymbol{s}(q^1,q^2) + q^3\boldsymbol{n}(q^1,q^2), \quad (7)$$

with $\boldsymbol{n}$ being the unit vector which is perpendicular to S and q^3 coordinate representing the distance from S. In this embedded 3D space, the covariant components of the metric tensor read

$$G_{ij} = \partial_i\boldsymbol{x}\cdot\partial_j\boldsymbol{x}, \quad (i,j=1,2,3), \quad (8)$$

with ∂_i standing for the derivative with respect to the spatial variable q^i. The confining potential V_λ, which is assumed to be strong enough to localize the particle on surface S, can be described as an ideal potential that only depends on the normal coordinate q^3 and has the limitation

$$V_\lambda(q^3) = \begin{cases} 0, & q^3 = 0, \\ \infty, & q^3 \neq 0. \end{cases} \quad (9)$$

Similarly, the background potential $V_{\rm s}$ can be parameterized as $V_{\rm s}(q^1, q^2)$. Taking into account the geometry of the space, we expand Eq. (6) in the curvilinear coordinates by covariant calculus as

$$i\hbar\frac{\partial}{\partial t}\Psi(t,\boldsymbol{q}) = \frac{-\hbar^2}{2m}\sqrt{G}^{-1}\partial_i(\sqrt{G}G^{ij}\partial_j\Psi(t,\boldsymbol{q})) + i\hbar G^{ij}\Omega_i\partial_j\Psi(t,\boldsymbol{q}) + V_{\rm s}(q^1,q^2)\Psi(t,\boldsymbol{q}) + V_\lambda(q^3)\Psi(t,\boldsymbol{q}), \quad (10)$$

where G^{ij} is the inverse of metric tensor G_{ij}, $G = \det(G_{ij})$, $\Omega_a = \boldsymbol{\Omega}\cdot\partial_a\boldsymbol{s}/|\partial_a\boldsymbol{s}|(a=1,2)$, and $\Omega_3 = \Omega\cdot\boldsymbol{n}$. In this work, the Einstein summation convention is adopted. The 2D reduced metric tensor on S is defined as $g_{ab} = \partial_a\boldsymbol{s}\cdot\partial_b\boldsymbol{s}$, $(a,b=1,2)$. The relations between G_{ij} and g_{ab} are

$$\begin{aligned} G_{ab} &= g_{ab} + [\alpha g + (\alpha g)^{\mathrm{T}}]_{ab}q^3 + (\alpha g\alpha^{\mathrm{T}})_{ab}(q^3)^2, \\ G_{a3} &= G_{3a} = 0, \quad G_{33} = 1, \end{aligned} \tag{11}$$

where $(\alpha g)_{ab} = \alpha^c_a g_{cb}$, and α^c_a is the Weingarten curvature matrix which yields the Gauss–Weingarten equations[29,30]

$$\begin{aligned} \partial_a\partial_b\boldsymbol{s} &= \Gamma^c_{ab}\partial_c\boldsymbol{s} + h_{ab}\boldsymbol{n}, \\ \partial_a\boldsymbol{n} &= \alpha^b_a\partial_b\boldsymbol{s} = -h_{ac}g^{cb}\partial_b\boldsymbol{s}, \end{aligned} \tag{12}$$

with Γ^c_{ab} being the Christoffel symbols, g^{cb} the inverse of (g_{cb}), and h_{ac} the coefficients of second fundamental form of the surface S. The determinant of reduced metric tensor g_{ab} is represented by g, and the relation between G and g yields

$$G = f^2 g, \tag{13}$$

with $f = 1 + \mathrm{tr}(\alpha)q^3 + \det(\alpha)(q^3)^2$.

In contrast to the previous studies concerned,[8,10] one cannot directly decouple $\Psi(t,\boldsymbol{q})$ in Eq. (10) into the normal and tangential parts completely by applying the thin-layer procedure due to the coupling between Ω_3 and $\partial_3\Psi$. Fortunately, since $\Omega_3 = \Omega\cdot\boldsymbol{n} = [\boldsymbol{\omega}\times(\boldsymbol{s}+q^3\boldsymbol{n})]\cdot\boldsymbol{n} = \boldsymbol{\omega}\times\boldsymbol{s}\cdot\boldsymbol{n}$, the normal component of Coriolis factor Ω_3 is just functionally dependent on (q^1,q^2). Here we can introduce a gauge transformation with new wave function $\phi(t,q)$,

$$\Psi(t,\boldsymbol{q}) = \exp\left[\frac{i}{\hbar}m\Omega_3(q^1,q^2)q^3\right]\phi(t,\boldsymbol{q}), \tag{14}$$

for eliminating $i\hbar\Omega^3\partial_3\Psi$. The expression of the metric tensor given in Eq. (11) suggests that the Schrödinger equation with gauge transformation (14) can be separated into a surface part and a normal part. We follow the well-established thin-layer quantization procedure and introduce the separated wave function

$$\chi(t,\boldsymbol{q}) = \chi_{\mathrm{s}}(t,q^1,q^2)\chi_n(t,q^3) = \sqrt{f}\phi(t,\boldsymbol{q}), \tag{15}$$

as da Costa[8] with $\chi_{\mathrm{s}}(t,q^1,q^2)$ and $\chi_n(t,q^3)$ standing for the surface component and the normal component of wave function, respectively. Substituting Eqs. (14) and (15) into Eq. (10), in the limit where the thickness goes to zero, we obtain

$$\begin{aligned} i\hbar\frac{\partial}{\partial t}\chi = &-\frac{\hbar^2}{2m}\sqrt{g}^{-1}\partial_a(\sqrt{g}g^{ab}\partial_b\chi) - \frac{\hbar^2}{2m}\partial_3^2\chi \\ &-\frac{i\hbar\Omega_3(\mathrm{tr}\alpha)}{2}\chi - \frac{\hbar^2}{2m}\Big[\frac{1}{4}(\mathrm{tr}(\alpha))^2 \\ &-\det(\alpha)\Big]\chi + i\hbar g^{ab}\Omega_a\partial_b\chi \\ &-\frac{m\Omega_3^2}{2}\chi + V_\lambda(q^3)\chi + V_{\mathrm{s}}(q^1,q^2)\chi. \end{aligned} \tag{16}$$

From Eq. (16), it is easily seen that there is no coupling between Ω_3 and $\partial_3\chi$. The terms that only depend on normal coordinate q^3 or on surface coordinates (q^1,q^2) form the fast and slow quantum degrees of freedom. Equation (16) can be decoupled into independent normal and surface Schrödinger equations as

$$i\hbar\frac{\partial}{\partial t}\chi_n = \frac{-\hbar^2}{2m}\partial_3^2\chi_n + V_\lambda\chi_n, \tag{17}$$

$$\begin{aligned} i\hbar\frac{\partial}{\partial t}\chi_{\mathrm{s}} = &\frac{-\hbar^2}{2m}\frac{1}{\sqrt{g}}\partial_a[\sqrt{g}g^{ab}\partial_b\chi_{\mathrm{s}}] + V_{\mathrm{g}}\chi_{\mathrm{s}} \\ &+\Big(\frac{-i\hbar\Omega_3(\mathrm{Tr}(\alpha))}{2} - \frac{m\Omega_3^2}{2}\Big)\chi_{\mathrm{s}} \\ &+ i\hbar g^{ab}\Omega_a\partial_b\chi_{\mathrm{s}} + V_{\mathrm{s}}\chi_{\mathrm{s}}, \end{aligned} \tag{18}$$

with $V_{\mathrm{g}} = \frac{-\hbar^2}{2m}\Big[\frac{1}{4}(\mathrm{tr}(\alpha))^2 - \det(\alpha)\Big]$ being the well-known geometric potential. Equation (17) is the normal Schrödinger equation of a particle confined by the squeezing potential $V_\lambda(q^3)$. This expression is analogous to the results of other researchers in the perpendicular orientation,[8,10] while we would like to claim that the wave function decoupled here is $\phi(t,\boldsymbol{q})$, and χ_n is identified with da Costa's normal wave function just in the limit $q^3\to 0$.[8] Equation (18) describes the quantum dynamics of a particle bounded to the rotating surface S in the presence of Coriolis effects. The tangential Coriolis terms $\Omega_{1,2}$ are coupled with the surface geometric metric tensor and the tangential momentum operator, while the normal Coriolis term Ω_3 is coupled with the surface mean curvature and the mass of particle. In addition to the well-known geometric potential, the terms induced by the Coriolis effect, $-i\Omega_3\frac{\mathrm{tr}\alpha}{2} - m\frac{\Omega_3^2}{2}$, form a novel non-inertial potential which we call the Coriolis-induced geometric potential. The imaginary part of this potential $-i\Omega_3\mathrm{tr}\frac{\alpha}{2}$ does not vanish in the general case which gives rise to the loss of the Hermiticity and extends the study of this system to the field of Non-Hermitian quantum dynamics.[31,32] However, the imaginary term would be eliminated under two special conditions with respect to the geometry of the curved surface S. First, the mean curvature of S equals zero, which means that the rotating surface S is a minimal surface, such as plane or catenoid. Secondly, Ω_3 vanishes, which means that $\boldsymbol{\Omega}$ is perpendicular to $\boldsymbol{n}$ everywhere. Logically, Ω_3 identically equals zero on S only if the surface is axial symmetry about its rotational axis. The non-Hermitian term in surface Hamiltonian, resulting from the Coriolis effect and the confining procedure, stands for not only an additive equivalent term in the co-rotational frame but also the interaction between the confining particles and the environment. It is worth noting that the surface Schrödinger equation with the Coriolis effect (Eq. (18)) is reduced to the usual surface Schrödinger equation presented in Ref. [8] when the angular speed vanishes, as is expected.

In conclusion, we have studied the quantum dynamics of a spin-less particle constrained to move on a 2D curved surface S rotating around a fixed axis. In the co-rotational reference X' attached to S, the Coriolis effect has been introduced to present the equivalent Schrödinger equation. Due to the coupling between Ω_3 and $\partial_3\Psi$, one cannot separate Eq. (10) into the normal and the surface components directly. We have introduced a proper gauge transformation for wave function Ψ in Eq. (14), which has eliminated this coupling term and made the JKC scheme still available in the rotating system. It is worth noting that the new wave function ϕ, employed in Eq. (14), is identical to Ψ in the limitation where q^3 goes to zero. In consideration of both the gauge transform wave function and the separated wave function (15), we have obtained the Schrödinger equation in the co-rotational curvilinear coordinates with the zeroth order of q^3 (in the limit of $q^3 \to 0$), and decoupled the Schrödinger equation into the normal and the surface components as da Costa. In the surface Schrödinger equation, the tangential Coriolis terms are coupled with the surface geometric metric tensor and the tangential momentum operator, while the well-known geometric potential has been obtained with its form unchanged. Moreover, the Coriolis-induced geometric potential, $-i\Omega_3(\mathrm{tr}(\alpha))/2 - m\Omega_3^2/2$, has been obtained. In this effective potential, the normal part of the Coriolis factor Ω_3 is coupled with the surface curvature which leads to a non-Hermitian Hamiltonian. We have speculated that this non-Hermitian term vanishes when the rotating curved surface is a minimal surface or a revolution surface that is axial symmetric about the rolling axis. It is easily seen that we have discussed the general case of the quantum dynamics of a non-relativistic particle constrained on a rotating curved surface and shown the quantum behavior modified by the action resulting from both the geometry and the Coriolis effect on a nano rotator.

Finally, for smoothly reading, we give the time-spatial transformation from X to X'. In the co-rotational frame X' aforementioned, the position vector can be expanded by coordinates x^i as $x^i\boldsymbol{e}'_i$ with $i = 1, 2, 3$, where x^i is functionally dependent on τ while wave function in X' can be rewritten as $\Psi[t(\tau), \boldsymbol{x}(\tau, \boldsymbol{r})]$. The transformation of time derivative reads

$$\begin{aligned}\frac{\partial}{\partial\tau} &= \frac{\partial t}{\partial\tau}\frac{\partial}{\partial t} + \frac{\partial x^i}{\partial\tau}\frac{\partial}{\partial x^i}\\ &= \frac{\partial}{\partial t} + r^k\partial_\tau(R_{ik})\frac{\partial}{\partial x^i}\\ &= \frac{\partial}{\partial\tau} + x^s\partial_\tau(R_{ik})R^{-1}_{ks}\frac{\partial}{\partial x^i},\end{aligned} \tag{19}$$

with R indicating a proper rotation transformation matrix which satisfies

$$\begin{pmatrix} x_1\\ x_2\\ x_3\end{pmatrix} = [R]\begin{pmatrix} r_1\\ r_2\\ r_3\end{pmatrix}. \tag{20}$$

Analogously, the gradient operator is transformed as

$$\begin{aligned}\nabla_{\boldsymbol{r}} &= \boldsymbol{e}_i\frac{\partial}{\partial r^i} = \boldsymbol{e}'_j R_{ji}\frac{\partial x^k}{\partial r^i}\frac{\partial}{\partial x^k}\\ &= \boldsymbol{e}'_j R_{ji}R_{ki}\frac{\partial}{\partial x^k} = \boldsymbol{e}'_i\frac{\partial}{\partial x^i} = \nabla_{\boldsymbol{x}}.\end{aligned} \tag{21}$$

When the surface S rotates around $\boldsymbol{e}_3(\boldsymbol{e}'_3)$ with angular velocity ω, the transformed matrix R can be written explicitly as

$$R = \begin{pmatrix} \cos(\omega\tau) & \sin(\omega\tau) & 0\\ -\sin(\omega\tau) & \cos(\omega\tau) & 0\\ 0 & 0 & 1\end{pmatrix}. \tag{22}$$

We substitute the equation above into Eq. (19) and obtain

$$\frac{\partial}{\partial\tau} = \frac{\partial}{\partial t} + \omega\Big(x_2\frac{\partial}{\partial x_1} - x_1\frac{\partial}{\partial x_2}\Big) = \frac{\partial}{\partial t} - \frac{i}{\hbar}\omega\hat{L}_3, \tag{23}$$

with

$$\hat{L}_3 = i\hbar\Big(x_2\frac{\partial}{\partial x_1} - x_1\frac{\partial}{\partial x_2}\Big).$$

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