Berry phase and Dirac monopole

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We shall explore the similarity between the Lagrangian for a spin-$\frac{1}{2}$ in a magnetic field and that for a charged particle in a magnetic field encountered when we discussed the Aharonov-Bohm phase. We shall then discover the *Berry connection*, the *Berry curvature*, and the *Berry phase* from the former Lagrangian, which correspond to the vector potential, the magnetic field, and the Aharonov-Bohm phase, respectively, appeared from the latter Lagragian. It turns out that the Berry curvature describes the non-zero divergent field associated with a magnetic monopole, called the *Dirac monopole*. We shall then discuss the intimate relation between the Dirac monopole and quantization of spin.

I. BERRY CONNECTION, BERRY CURVATURE, AND BERRY PHASE

We found that the effective Lagrangian for the spin$-\frac{1}{2}$ in the magnetic field $\boldsymbol{B} = \begin{bmatrix} 0 \\ 0 \\ B \end{bmatrix}$ can be given by

$$\mathcal{L}(\phi, \dot{\phi}, \theta, \dot{\theta}) = \underbrace{\frac{1}{2}\gamma_s B \cos\theta}_{\text{potential energy}} + \underbrace{\frac{i}{2}\left(1 - \cos\theta\right)\dot{\phi}}_{\text{velocity dependent part}}, \tag{1}$$

This reminds us of the *imaginary-time* version of the Lagrangian for the charged particle in the vector potential $\boldsymbol{A}$, that is,

$$\mathcal{L}(\boldsymbol{x}, \dot{\boldsymbol{x}}) = \underbrace{\frac{1}{2}m\dot{\boldsymbol{x}}^2}_{\text{kinetic energy}} - \underbrace{iq\boldsymbol{A}\cdot\dot{\boldsymbol{x}}}_{\text{velocity dependent part}}, \tag{2}$$

since both Lagrangians contain the *velocity-dependent imaginary parts*. Let us take this analogy seriously and find the corresponding vector potential $\boldsymbol{A}$ for the former.

To this end let us remember that the Euler-Lagrange equation followed from the Lagrangian Eq. (1) is

$$\dot{\boldsymbol{n}} = -\gamma_s \boldsymbol{n} \times \boldsymbol{B}, \tag{3}$$

where the *normalized* magnetic moment $\boldsymbol{n} = \frac{\boldsymbol{m}}{m_0} = -2\boldsymbol{\sigma}$ ($\boldsymbol{m}$: magnetic moment; $m_0 = \frac{g\mu_B}{2}$) can be written in terms of two Euler angles as

$$\boldsymbol{n} = \begin{bmatrix} \sin\theta\cos\phi \\ \sin\theta\sin\phi \\ \cos\theta \end{bmatrix}, \tag{4}$$

with and the spherical orthonormal system:

$$\boldsymbol{e}_r = \begin{bmatrix} \sin\theta\cos\phi \\ \sin\theta\sin\phi \\ \cos\theta \end{bmatrix} \tag{5}$$

$$\boldsymbol{e}_\theta = \begin{bmatrix} \cos\theta\cos\phi \\ \cos\theta\sin\phi \\ -\sin\theta \end{bmatrix} \tag{6}$$

$$\boldsymbol{e}_\phi = \begin{bmatrix} -\sin\phi \\ \cos\phi \\ 0 \end{bmatrix}. \tag{7}$$

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Thus, we can consider

$$\dot{\boldsymbol{\sigma}} = -\frac{1}{2}\dot{\boldsymbol{n}} = -\frac{1}{2}\left(\dot{\theta}\boldsymbol{e}_\theta + \sin\theta\dot{\phi}\boldsymbol{e}_\phi\right) = -\frac{1}{2}\begin{bmatrix} 0 \\ \dot{\theta} \\ \sin\theta\dot{\phi} \end{bmatrix}, \tag{8}$$

as the more proper velocity for the spin moving on a sphere with radius of $\frac{1}{2}$. The velocity-dependent imaginary part of the Lagrangian $\mathcal{L}(\phi, \dot{\phi}, \theta, \dot{\theta})$ in Eq. (1) can thus be rewritten in a very similar way as the corresponding part of Eq. (2) as

$$\mathcal{L}_B(\phi, \dot{\phi}, \theta, \dot{\theta}) \equiv \frac{i}{2}\left(1-\cos\theta\right)\dot{\phi} = -i\boldsymbol{A}_\uparrow \cdot \dot{\boldsymbol{\sigma}}, \tag{9}$$

where we defined the vector-potential-like quantity $\boldsymbol{A}_\uparrow$ as

$$\boldsymbol{A}_\uparrow = \begin{bmatrix} 0 \\ 0 \\ \frac{1-\cos\theta}{\sin\theta} \end{bmatrix} \tag{10}$$

in the spherical coordinates. This vector potential is called the *Berry connection* in the literature [1]. The subscript $\uparrow$ emphasizes the fact that the Berry connection stems from the *state* $|\uparrow\rangle$, which we shall see more later on.

The *Berry phase action* can thus be written in three different ways:

$$S_{\text{top}}[\phi,\theta] = -\int_0^\beta d\tau \left\langle \frac{\partial}{\partial\tau} g \middle| g \right\rangle \tag{11}$$

$$= \frac{i}{2}\int_0^\beta d\tau \left(1-\cos\theta\right)\dot{\phi} \tag{12}$$

$$= -i\int_0^\beta d\tau \boldsymbol{A}_\uparrow \cdot \dot{\boldsymbol{\sigma}}. \tag{13}$$

Now we shall find the another expression of the Berry connection $\boldsymbol{A}_\uparrow$. First, notice that

$$\frac{\partial}{\partial\tau}\langle g|g\rangle = \left\langle \frac{\partial}{\partial\tau} g \middle| g \right\rangle + \left\langle g \middle| \frac{\partial}{\partial\tau} g \right\rangle = 0 \tag{14}$$

and thus

$$\left\langle \frac{\partial}{\partial\tau} g \middle| g \right\rangle = -\left\langle g \middle| \frac{\partial}{\partial\tau} g \right\rangle \tag{15}$$

and $\left\langle g \middle| \frac{\partial}{\partial\tau} g \right\rangle$ is pure imaginary. Equation. (11) can thus be rewritten as

$$S_{\text{top}}[\phi,\theta] = \int_0^\beta d\tau \left\langle g \middle| \frac{\partial}{\partial\tau} g \right\rangle. \tag{16}$$

Next, notice $g(\tau)$, a function of τ, can also be viewed as $g(\boldsymbol{\sigma}(\tau))$, a function of $\boldsymbol{\sigma}(\tau)$, that is,

$$S_{\text{top}}[\phi,\theta] = \int_0^\beta d\tau \left\langle g(\boldsymbol{\sigma}(\tau)) \middle| \frac{\partial}{\partial\boldsymbol{\sigma}(\tau)} g(\boldsymbol{\sigma}(\tau)) \right\rangle \dot{\boldsymbol{\sigma}}(\tau). \tag{17}$$

Comparing this expression with Eq. (13) we find the more famous expression of the Berry connection:

$$\boldsymbol{A}_\uparrow = i\left\langle g(\boldsymbol{\sigma}) \middle| \frac{\partial}{\partial\boldsymbol{\sigma}} \middle| g(\boldsymbol{\sigma}) \right\rangle, \tag{18}$$

which, from Eq. (15), is a real-valued quantity.

Let us find some more. Since the integration with respect to τ in Eq.(13) running from $\tau = 0$ to β is traded for the contour integration with respect to $\boldsymbol{\sigma}$, the Berry phase action can be further modified to

$$\begin{aligned} S_{\text{top}}[\phi,\theta] &= -i\oint_{\mathcal{C}} \boldsymbol{A}_\uparrow \cdot d\boldsymbol{\sigma} \\ &= -i\int_{\mathcal{A}} \underbrace{(\boldsymbol{\nabla}\times\boldsymbol{A}_\uparrow)}_{\boldsymbol{\Omega}_\uparrow} \cdot d\boldsymbol{S}, \end{aligned} \tag{19}$$

using Stokes theorem, where $\int_C d\boldsymbol{\sigma}$ is the contour integral with respect to $\boldsymbol{\sigma}$ along the circle $\mathcal{C}$ while $\int_\mathcal{A} d\boldsymbol{S}$ is the surface integral over the area $\mathcal{A}$ bounded by the circle $\mathcal{C}$. Here,

$$\boldsymbol{\Omega}_\uparrow = \boldsymbol{\nabla} \times \boldsymbol{A}_\uparrow \tag{20}$$

is like magnetic field and is called the *Berry curvature* in the literature [1].

Like a charged particle moving in a ring, which is threaded by a magnetic field $\boldsymbol{B}$, acquires the Aharonov-Bohm phase, the magnetic moment moving on the sphere with the Berry curvature $\boldsymbol{\Omega}_\uparrow$ acquires the *Berry phase* $\gamma_\uparrow$, which is defined by

$$\gamma_\uparrow = \oint_\mathcal{C} d\boldsymbol{\sigma} \cdot \boldsymbol{A}_\uparrow = \int_\mathcal{A} d\boldsymbol{S} \cdot \boldsymbol{\Omega}_\uparrow. \tag{21}$$

We have thus the following correspondences:

$$\begin{array}{lcl} \text{vector potential} : \boldsymbol{A} & \Leftrightarrow & \text{Berry connection} : \boldsymbol{A}_\uparrow \\ \text{magnetic field} : \boldsymbol{B} = \boldsymbol{\nabla} \times \boldsymbol{A} & \Leftrightarrow & \text{Berry curvature} : \boldsymbol{\Omega}_\uparrow = \boldsymbol{\nabla} \times \boldsymbol{A}_\uparrow \\ \text{Aharonov} - \text{Bohm phase} : \gamma & \Leftrightarrow & \text{Berry phase} : \gamma_\uparrow \end{array} .$$

II. DIRAC MONOPOLE

A. Dirac monopole [2]

Now let us explore the Berry connection $\boldsymbol{A}_\uparrow$ and the Berry curvature $\boldsymbol{\Omega}_\uparrow$ a little bit more. According to the above argument, the Berry curvature $\boldsymbol{\Omega}_\uparrow$ is like magnetic field. Then what kind of magnetic field? Taking rotation of $\boldsymbol{A}_\uparrow$ given by Eq. (10) in the spherical coordinate system $(r = \frac{1}{2}, \theta, \phi)$ we have

$$\begin{aligned} \boldsymbol{\Omega}_\uparrow &= \boldsymbol{\nabla} \times \boldsymbol{A}_\uparrow \\ &= \left(\boldsymbol{e}_r \frac{\partial}{\partial r} + \boldsymbol{e}_\theta \frac{1}{r} \frac{\partial}{\partial \theta} + \boldsymbol{e}_\phi \frac{1}{r \sin\theta} \frac{\partial}{\partial \phi} \right) \times (A_r \boldsymbol{e}_r + A_\theta \boldsymbol{e}_\theta + A_\phi \boldsymbol{e}_\phi) \\ &= \left(\boldsymbol{e}_r \frac{\partial}{\partial r} + \boldsymbol{e}_\theta \frac{1}{\frac{1}{2}} \frac{\partial}{\partial \theta} + \boldsymbol{e}_\phi \frac{1}{\frac{1}{2}\sin\theta} \frac{\partial}{\partial \phi} \right) \times \left(\frac{1-\cos\theta}{\sin\theta} \boldsymbol{e}_\phi \right) \\ &= \begin{bmatrix} \frac{1}{\frac{1}{2}\sin\theta} \frac{\partial}{\partial\theta} (\sin\theta A_\phi) - \frac{\partial}{\partial\phi} A_\theta \\ \frac{1}{\frac{1}{2}\sin\theta} \frac{\partial}{\partial\phi} A_r - \frac{1}{\frac{1}{2}} \frac{\partial}{\partial r} \left(\frac{1}{2} A_\phi \right) \\ \frac{1}{\frac{1}{2}} \frac{\partial}{\partial r} \left(\frac{1}{2} A_\theta \right) - \frac{1}{\frac{1}{2}} \frac{\partial}{\partial\theta} A_r \end{bmatrix} = \begin{bmatrix} 2 \\ 0 \\ 0 \end{bmatrix} \\ &= 2\boldsymbol{e}_r, \end{aligned} \tag{22}$$

where we use $\boldsymbol{\nabla}$ in the spherical coordinate system (see Appendix A for the derivation),

$$\boldsymbol{\nabla} = \boldsymbol{e}_r \frac{\partial}{\partial r} + \boldsymbol{e}_\theta \frac{1}{r} \frac{\partial}{\partial \theta} + \boldsymbol{e}_\phi \frac{1}{r \sin\theta} \frac{\partial}{\partial \phi}, \tag{23}$$

and the following relations:

$$\boldsymbol{e}_i \cdot \boldsymbol{e}_j = \delta_{ij} \tag{24}$$

$$\boldsymbol{e}_i \times \boldsymbol{e}_j = \epsilon_{ijk} \boldsymbol{e}_k \tag{25}$$

$$\frac{\partial}{\partial r} \begin{bmatrix} \boldsymbol{e}_r \\ \boldsymbol{e}_\theta \\ \boldsymbol{e}_\phi \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix} \tag{26}$$

$$\frac{\partial}{\partial \theta} \begin{bmatrix} \boldsymbol{e}_r \\ \boldsymbol{e}_\theta \\ \boldsymbol{e}_\phi \end{bmatrix} = \begin{bmatrix} \boldsymbol{e}_\theta \\ -\boldsymbol{e}_r \\ 0 \end{bmatrix} \tag{27}$$

$$\frac{\partial}{\partial \phi} \begin{bmatrix} \boldsymbol{e}_r \\ \boldsymbol{e}_\theta \\ \boldsymbol{e}_\phi \end{bmatrix} = \begin{bmatrix} \sin\theta \boldsymbol{e}_\phi \\ \cos\theta \boldsymbol{e}_\phi \\ -\sin\theta \boldsymbol{e}_r - \cos\theta \boldsymbol{e}_\theta \end{bmatrix}. \tag{28}$$

Notice that Eq. (22) suggests that the magnetic field is pointing radially, just like the *magnetic monopole*! This monopole is called the *Dirac monopole* in some literature [3]. The strange point of the Dirac monopole is that the divergence of the field $\boldsymbol{\Omega}_\uparrow = 8$ and is not zero. This means that the Berry connection $\boldsymbol{A}_\uparrow$ should be ill-behaved since $\boldsymbol{\nabla} \cdot (\boldsymbol{\nabla} \times \boldsymbol{A}_\uparrow) \neq 0$. This is indeed true. $A_\phi = \frac{1-\cos\theta}{\sin\theta} = \tan\frac{\theta}{2}$ is singular at $\theta = \pi$ as seen in Fig. 1.

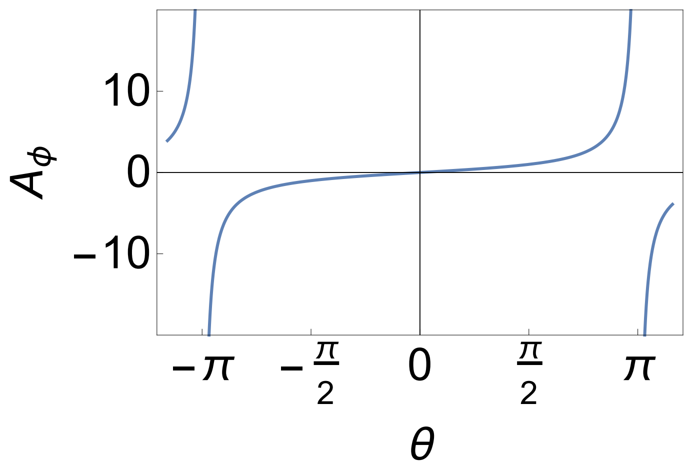

FIG. 1. ϕ-component of Berry connection $\boldsymbol{A}_\uparrow$, $A_\phi = \frac{1-\cos\theta}{\sin\theta} = \tan\frac{\theta}{2}$, as a function of θ.

We could partly remedy this situation by using the other Berry connection, for instance,

$$\boldsymbol{A}_\downarrow = \begin{bmatrix} 0 \\ 0 \\ -\frac{1+\cos\theta}{\sin\theta} \end{bmatrix}, \tag{29}$$

which can be obtained by the following gauge transformation:

$$\begin{aligned} \boldsymbol{A}_\downarrow &= \boldsymbol{A}_\uparrow - \boldsymbol{\nabla}\phi \\ &= \boldsymbol{A}_\uparrow - \left(\boldsymbol{e}_r \frac{\partial}{\partial r} + \boldsymbol{e}_\theta \frac{1}{\frac{1}{2}} \frac{\partial}{\partial \theta} + \boldsymbol{e}_\phi \frac{1}{\frac{1}{2}\sin\theta} \frac{\partial}{\partial \phi} \right) \phi \\ &= \begin{bmatrix} 0 \\ 0 \\ \frac{1-\cos\theta}{\sin\theta} \end{bmatrix} - \begin{bmatrix} 0 \\ 0 \\ \frac{1}{\frac{1}{2}\sin\theta} \end{bmatrix}. \end{aligned} \tag{30}$$

Like vector potentials, the Berry connection is thus gauge-dependent. The gauge-transformed Berry connection $\boldsymbol{A}_\downarrow$ in Eq. (29) does not have singularity at $\theta = \pi$, but does have it at $\theta = 0$ as seen in Fig. 2. Note that the Berry connection $\boldsymbol{A}_\downarrow$ produces exactly the same Berry curvature $\boldsymbol{\Omega}_\downarrow$ as $\boldsymbol{\Omega}_\uparrow$ in Eq. (22), thus, like magnetic field, the Berry curvature is gauge-independent.

What about the Berry phase $\gamma_\uparrow$ in Eq. (21)? Does it change by the gauge transformation Eq. (30)? Let us see the interesting answer to this question. Remember that $\boldsymbol{\sigma}$ in Eq. (21) traverses the circle $\mathcal{C}$ on the sphere of radius $\frac{1}{2}$. Let us suppose the area $\mathcal{A}$ enclosed by $\mathcal{C}$ is $A_{\mathcal{C},\uparrow}$ when the area contains the north pole and $A_{\mathcal{C},\downarrow}$ when the area contains the south pole. The Berry phase can then be given by this area $A_{\mathcal{C},\uparrow}$ as

$$\gamma_\uparrow = \int_{\mathcal{A}_\uparrow} d\boldsymbol{S} \cdot \boldsymbol{\Omega}_\uparrow = \int_{\mathcal{A}_\uparrow} d\boldsymbol{S} \cdot 2\boldsymbol{e}_r = 2A_{\mathcal{C},\uparrow} \tag{31}$$

while it can be given by $A_{\mathcal{C},\downarrow}$ as

$$\gamma_\downarrow = \int_{\mathcal{A}_\downarrow} d\boldsymbol{S} \cdot \boldsymbol{\Omega}_\downarrow = \int_{\mathcal{A}_\downarrow} d\boldsymbol{S} \cdot 2\boldsymbol{e}_r = -2A_{\mathcal{C},\downarrow}, \tag{32}$$

where the minus sign comes from the fact that the area here has the *orientation* with respect to the circle $\mathcal{C}$. Are these two expressions different? To see this, let us calculate the difference:

$$\gamma_\uparrow - \gamma_\downarrow = 2A_{\mathcal{C},\uparrow} + 2A_{\mathcal{C},\downarrow} = 2 \underbrace{4\pi\left(\frac{1}{2}\right)^2}_{\text{sphere surface of radius}\frac{1}{2}} = 2\pi. \tag{33}$$

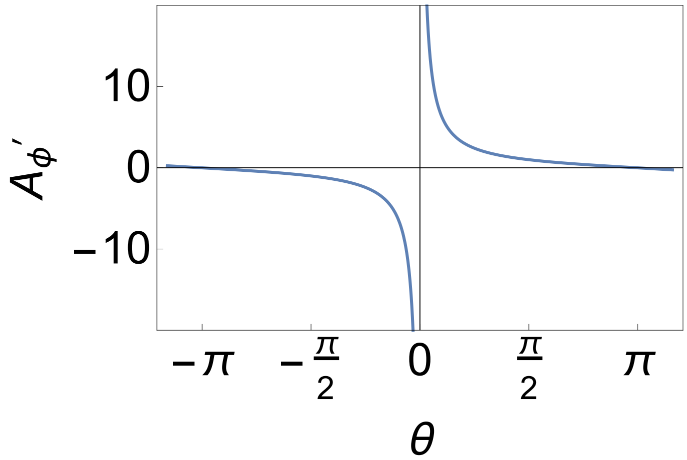

FIG. 2. ϕ-component of Berry connection $\boldsymbol{A}_\downarrow$, $A'_\phi = -\frac{1+\cos\theta}{\sin\theta} = \frac{1}{\tan\frac{\theta}{2}}$, as a function of θ.

Thus the answer is no in a sense of modulo 2π! We thus say that $\gamma_\uparrow = \gamma_\downarrow$ and the the Berry phase is gauge-independent!

B. Quntization of spin [2]

We can repeat the similar arguments for the general spin-S cases to reach the conclusion that the Berry phase acquired by the spin-S moving on sphere of radius S is

$$\gamma_\uparrow = \frac{1}{S} A_{\mathcal{C},\uparrow} \tag{34}$$

for the calcuration based on the area contains the north pole while

$$\gamma_\downarrow = -\frac{1}{S} A_{\mathcal{C},\downarrow} \tag{35}$$

for that based on the area contains the south pole. The difference is thus given by

$$\gamma_\uparrow - \gamma_\downarrow = \frac{1}{S} A_{\mathcal{C},\uparrow} + \frac{1}{S} A_{\mathcal{C},\downarrow} = \frac{1}{S} \underbrace{4\pi S^2}_{\text{sphere surface of radius} S} = 4\pi S. \tag{36}$$

We can thus draw a very interesting conclusion that as far as the spin is quantized as $\frac{1}{2}, 1, \frac{3}{2}, \cdots$, the Berry phase can be single-valued (modulo 2π) and gauge-independent. It also seen that the minimum possible spin is not 1 but $\frac{1}{2}$!

This in turn means that *the spin has to be quantized if we require that the Berry phase is single-valued (modulo 2π)!* We can see (again) the close link between the topological phase and quantized quantity, constituting a yet another correspondence

$$\text{Flux quantization} \;\Leftrightarrow\; \text{Spin quantization}\ .$$

Appendix A: ∇ in the spherical coordinate system

In the spherical coordinate system, we have

$$x = r\sin\theta\cos\phi \tag{A1}$$
$$y = r\sin\theta\cos\phi \tag{A2}$$
$$z = r\cos\theta. \tag{A3}$$

This leads to the following relationship between (dx, dy, dz) and $(dr, d\theta, d\phi)$:

$$\begin{bmatrix} dx \\ dy \\ dz \end{bmatrix} = \begin{bmatrix} \frac{\partial x}{\partial r} & \frac{\partial x}{\partial \theta} & \frac{\partial x}{\partial \phi} \\ \frac{\partial y}{\partial r} & \frac{\partial y}{\partial \theta} & \frac{\partial y}{\partial \phi} \\ \frac{\partial z}{\partial r} & \frac{\partial z}{\partial \theta} & \frac{\partial z}{\partial \phi} \end{bmatrix} \begin{bmatrix} dr \\ d\theta \\ d\phi \end{bmatrix} = \begin{bmatrix} \sin\theta\cos\phi & r\cos\theta\cos\phi & -r\sin\theta\sin\phi \\ \sin\theta\sin\phi & r\cos\theta\sin\phi & r\sin\theta\cos\phi \\ \cos\theta & -r\sin\theta & 0 \end{bmatrix} \begin{bmatrix} dr \\ d\theta \\ d\phi \end{bmatrix}. \tag{A4}$$

This, in turn, brings us to

$$\begin{aligned} \boldsymbol{\nabla} = \begin{bmatrix} \frac{\partial}{\partial x} \\ \frac{\partial}{\partial y} \\ \frac{\partial}{\partial z} \end{bmatrix} = \begin{bmatrix} \frac{\partial r}{\partial x} & \frac{\partial \theta}{\partial x} & \frac{\partial \phi}{\partial x} \\ \frac{\partial r}{\partial y} & \frac{\partial \theta}{\partial y} & \frac{\partial \phi}{\partial y} \\ \frac{\partial r}{\partial z} & \frac{\partial \theta}{\partial z} & \frac{\partial \phi}{\partial z} \end{bmatrix} \begin{bmatrix} \frac{\partial}{\partial r} \\ \frac{\partial}{\partial \theta} \\ \frac{\partial}{\partial \phi} \end{bmatrix} &= \begin{bmatrix} \sin\theta\cos\phi & \frac{1}{r}\cos\theta\cos\phi & -\frac{1}{r\sin\theta}\sin\phi \\ \sin\theta\sin\phi & \frac{1}{r}\cos\theta\sin\phi & \frac{1}{r\sin\theta}\cos\phi \\ \cos\theta & -\frac{1}{r}\sin\theta & 0 \end{bmatrix} \begin{bmatrix} \frac{\partial}{\partial r} \\ \frac{\partial}{\partial \theta} \\ \frac{\partial}{\partial \phi} \end{bmatrix} \\ &= \begin{bmatrix} \sin\theta\cos\phi & \cos\theta\cos\phi & -\sin\phi \\ \sin\theta\sin\phi & \cos\theta\sin\phi & \cos\phi \\ \cos\theta & -\sin\theta & 0 \end{bmatrix} \begin{bmatrix} \frac{\partial}{\partial r} \\ \frac{1}{r}\frac{\partial}{\partial \theta} \\ \frac{1}{r\sin\theta}\frac{\partial}{\partial \phi} \end{bmatrix} \\ &= [\boldsymbol{e}_r, \boldsymbol{e}_\theta, \boldsymbol{e}_\phi] \begin{bmatrix} \frac{\partial}{\partial r} \\ \frac{1}{r}\frac{\partial}{\partial \theta} \\ \frac{1}{r\sin\theta}\frac{\partial}{\partial \phi} \end{bmatrix} \\ &= \left(\boldsymbol{e}_r \frac{\partial}{\partial r} + \boldsymbol{e}_\theta \frac{1}{r}\frac{\partial}{\partial \theta} + \boldsymbol{e}_\phi \frac{1}{r\sin\theta}\frac{\partial}{\partial \phi} \right). \end{aligned} \tag{A5}$$

[1] D. Xiao, M. -C. Chang, and Q. Niu, Rev. Mod. Phys. **82**, 1959 (2010).
[2] A. Altland and B. D. Simons, *Condensed Matter Field Theory*, 2nd ed. (Cambridge University Press, Cambridge, 2010).
[3] J. J. Sakurai, *Modern Quantum Mechanics*, revised ed. (Addison-Wesley, Reading, MA, 1994).