An introduction to geometrical phases

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(Dated: September 20, 2019)

In their simplest form, geometrical phases are phases that accompany slow variation of external parameters. Since their discovery, these phases have found applications that go significantly beyond interference effects, influencing fields ranging from condensed matter physics and optics to high-energy physics, and even pure mathematics. In this article we give a pedagogical introduction to general geometric phases, with an accent on mathematical formalism.

I. INTRODUCTION

In his landmark article of 1984 Michael Berry studied the geometric phase that accompanied adiabatic evolution of a quantum system – a non-trivial phase that cannot be integrated out by a change of phase of the underlying state-space and thus has direct physical consequences on the things that we measure [1]. This phase has since then been generalized, sheding light on the geometrical mathematical structure of quantum mechanics, and found numerous applications in the Born-Oppenheimer approximation and molecular dynamics, Aharonov-Bohm effect, fluid dynamics, Modern Polarization Theory, semiclassical dynamics of electrons in metals and semiconductors, fractional statistics, quantized Hall effect, topological order, and many more.

Preceding Berry by three decades, Pancharatnam [2] was the first to study a geometrical phase in the context of optics; he studied the additional phase that polarized light acquires after a cyclic series of polarization changes. Aharonov and Bohm [3] in their famous article of 1959 discovered how in quantum mechanics even a vanishing magnetic field can influence the phase of the wave function. This is, in fact, a special type of geometrical phase. In molecular dynamics, Mead and Truhlar [4] five years before Berry expanded the standard Born-Oppenheimer treatment of molecules to include geometrical term that helped explain certain unaccounted boundary conditions and (geometrical) phases that appeared during previous studies of molecules.

Right after the discovery of Berry's phase, Simon [5] found a way to interpret this phase as a mathematically canonical connection on a principal U(1)-bundle over the parameter space. Berry's phase then becomes a holonomy of paths in parameter space. Wilczek and Zee [6] generalized Berry's phase to the case of a N-fold degenerate energy, in which the abelian U(1) phase become a non-abelian U(N) phase. Aharonov and Anandan [7] have studied geometrical phases on the projective Hilbert space, thus lifting the limitation of adiabatic evolution. Samuel and Bhandari [8] have found a canonical way of comparing the relative phases of non-orthogonal states.

Beyond the foundational discoveries and generalizations of the adiabatic phase described in the last paragraph, there has been a wealth of both practical applications in many fields and purely theoretical advances in the foundations of quantum mechanics. The practical applications we shall not attempt to review, and the interested reader we direct towards [16–21]. On the purely theoretical side, we will note that Kibble [9, 10] and Provost and Vallee [11] found a natural way to endow the projective Hilbert space with the structure of a Kähler manifold, i.e., with symplectic form, Riemannian metric, and almost complex form. A quantum geometric tensor whose real part is the metric of the projective Hilbert space, and imaginary part is Berry's curvature, is then canonically defined. All of these discoveries marked the beginning of Geometric Quantum Mechanics, reviewed in [12, 13], that is closely related to geometrical phases.

In this article we offer an introduction to the foundational discoveries of geometrical phases. In the first part of the paper, using only the most basic of knowledge about quantum mechanics and differential forms, we derive the central result of the theory. Some examples and applications are discussed in detail. In the second part of the paper, we introduce the more sophisticated mathematical formalism (almost) from scratch and apply it to the previous result. Our review draws heavily from [19–21], where the reader may find further topics of interest.

II. ADIABATIC EVOLUTION

The adiabatic theorem states that a physical system that starts in an eigenstate of the Hamiltonian remains in the corresponding eigenstate if we change the Hamiltonian slowly in time and if there is a gap between the energy of this eigenstate and the rest of the Hamiltonian's spectrum. During this adiabatic evolution of state of the system acquires a dynamical phase and a geometrical phase. In this section of the article, we shall study the adiabatic evolution in the simplest case of a nondegenerate eigenspace of the Hamiltonian. Along the way we shall prove the adiabatic theorem and derive the geometric phase that accompanies adiabatic evolution.

Let us imagine a physical system whose Hamiltonian $\hat{H}$ is a smooth function of external real parameters $R^\mu = (R^1, R^2, \ldots, R^N)$. We shall use Einstein's convention, where $\mu, \nu, \ldots$ are to be summed over $1, 2, \ldots, N$. For

any value of the parameters R^μ we can diagonalize this Hamiltonian:

$$\hat{H}(R^\mu)\,|k,R^\mu\rangle = E_k(R^\mu)\,|k,R^\mu\rangle\ , \tag{1}$$

thereby getting a complete orthonormal basis made of stationary states $\{|k,R^\mu\rangle\}_{k\in\mathbb{N}}$, that is here for the sake of simplicity assumed to be discreet. Both the eigenvectors and eigenvalues depend smoothly on R^μ.

Let us further suppose that the system is initially in a nondegenerate stationary state $|\psi(0)\rangle = |n\rangle$. If we now imagine slowly varying the parameters $R^\mu = R^\mu(t)$ in time $t \in [0,T]$, the system will evolve according to the Schrödinger equation:

$$\mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t}\,|\psi(t)\rangle = \hat{H}(R^\mu(t))\,|\psi(t)\rangle\ , \tag{2}$$

and in general it will not stay in its initial stationary state. If the variation of parameters is slow enough (something that will be quantified later), then we still expect the system to evolve approximately as if there is no time dependence in the Hamiltonian. This motivates the Ansatz:

$$|\psi(t)\rangle = \sum_k c_k(t)\mathrm{e}^{\mathrm{i}\vartheta_k(t)}\,|k,R^\mu(t)\rangle\ ,$$

with the dynamical phase factor defined as:

$$\vartheta_k(t) = -\frac{1}{\hbar}\int_0^t \mathrm{d}t'\,E_k(R^\mu(t'))\,,$$

and initial conditions $c_k(0) = \delta_{kn}$.

If we now plug this Ansatz in to the Schrödinger equation (2), act from the left with $\langle n|$, use the eigenvalue equation (1), and rearrange, we find out that:

$$\frac{\mathrm{d}c_n}{\mathrm{d}t} = -c_n\,\langle n|\frac{\mathrm{d}}{\mathrm{d}t}|n\rangle - \sum_{k\neq n} c_k\,\langle n|\frac{\mathrm{d}}{\mathrm{d}t}|k\rangle\,\mathrm{e}^{\mathrm{i}(\vartheta_k-\vartheta_n)}\,,$$

where the parameter and time dependencies have been suppressed, and the sum goes over the whole spectrum. We immediately see that the second term on the right-hand side in this equation is oscillatory with frequencies equal or larger than $\omega_g = E_g/\hbar$, which is determined by the energy gap E_g between the state $|n\rangle$ and the rest of the Hamiltonian spectrum. To estimate the contribution of this term, we differentiate the eigenvalue equation (1) in time and act on it from the left with $\langle n|$ for $k \neq n$, thus getting:

$$\langle n|\frac{\mathrm{d}}{\mathrm{d}t}|k\rangle = \frac{1}{E_k - E_n}\,\langle n|\frac{\mathrm{d}\hat{H}}{\mathrm{d}t}|k\rangle\ . \tag{3}$$

Now we see that for the second oscillatory term to be negligible the Hamiltonian has to change little compared to the energy gap E_g during one period $T_g = 2\pi/\omega_g$ in order to average out to zero. In other words, we demand that:

$$\left|\,\langle n|\frac{\mathrm{d}\hat{H}}{\mathrm{d}t}|k\rangle\right| \ll \omega_g E_g\ ,\ \text{for all } k \neq n.$$

This is the precise statement of the adiabatic limit. In the rest of the article, whenever we discuss adiabatic evolution of a physical system, we presume that this condition is satisfied.

A. Berry's phase

In this adiabatic limit the equation of motion for the c_n coefficient simplifies to:

$$\dot{c}_n = -c_n\,\langle n|\partial_\mu n\rangle\,\dot{R}^\mu\,,$$

which can easily be solved for c_n. Here overset dots mark time derivative, and $\partial_\mu = \partial/\partial R^\mu$. The normalization $\langle\varphi_n|\varphi_n\rangle = 1$ implies that $\langle\varphi_n|\partial_\mu\varphi_n\rangle$ is imaginary and that $c_n(t)$ has the form of a phase $\exp(\mathrm{i}\gamma_n(t))$. This is the *adiabatic* or *Berry's phase* $\gamma_n(t)$ – a non-dynamical phase that accompanies adiabatic evolution of eigenstates. By integrating the equations of motion, we can get an explicit expression for Berry's phase:

$$\gamma_n(t) = \mathrm{i}\int_0^t \mathrm{d}t'\,\frac{\mathrm{d}R^\mu}{\mathrm{d}t'}\,\langle n|\partial_\mu n\rangle\ . \tag{4}$$

Michael Berry was not the first to calculate this phase, for M. Born and V. Fock [14] preceded him by 55 years! But he was the first to note its physical significance. The reason this phase was ignored for so long was that a simple redefinition of the eigenvector appeared to eliminate it! In particular, there exists arbitrariness in choosing the eigenvectors $|n\rangle$ of the Hamiltonian: their phase. More formally, we can make an U(1) gauge transformation of the eigenvectors:

$$|n,R^\mu\rangle \longrightarrow \mathrm{e}^{\mathrm{i}\lambda_n(R^\mu)}\,|n,R^\mu\rangle\ , \tag{5}$$

which does not change anything physically. If using such a gauge transformation we can eliminate some phase then that phase cannot have any physical effect. As it turns out, whenever the final $R^\mu(T) = R^\mu_f$ and initial $R^\mu(0) = R^\mu_i$ parameters of the system are different we *can* in fact use the Born-Fock's gauge:

$$|n,R^\mu(t)\rangle \longrightarrow \mathrm{e}^{\mathrm{i}\gamma_n(t)}\,|n,R^\mu(t)\rangle\ ,$$

to eliminate the adiabatic phase. However, when $R^\mu_f = R^\mu_i$ then we *cannot* use Born-Fock's (or any other) gauge transformation to remove the adiabatic phase because one isn't allowed to gauge-transform the initial (= final) point in parameter space in two different ways.

Let us see how this works in more detail. To make progress we observe that in the explicit expression for Berry's phase (4) any reparameterization of the path $R^\mu(t)$ in parameter space does not change the value of the adiabatic phase. This allows us to reformulate Berry's phase as an integral of a 1-form over the path in parameter space. Let $\mathcal{C}$ be the oriented (future directed) path $R^\mu\colon [0,T] \to \mathbb{R}^N$ in parameter space, a let us define the

Berry's connection 1-form or *vector potential* of the n-th eigenvector as:

$$A_n(R^\mu) := \mathrm{i}\,\langle n|\mathrm{d}n\rangle = \mathrm{i}\,\langle n|\partial_\mu n\rangle\,\mathrm{d}R^\mu\ . \tag{6}$$

Now Berry's phase can be elegantly expressed as:

$$\gamma_n(\mathcal{C}) = \int_{\mathcal{C}} A_n\,.$$

To study how γ_n changes when we make a gauge transformation according to (5), we first determine how the Berry's 1-form changes. This can easily be determined by simply substituting (5) in to (6):

$$A_n(R^\mu) \longrightarrow A_n(R^\mu) - \mathrm{d}\lambda_n\,(R^\mu)\,.$$

The second term is simply the gradient of the gauge phase $\mathrm{d}\lambda_n = \partial_\nu\lambda_n(R^\mu)\,\mathrm{d}R^\nu$, which can be integrated out thus resulting in the following gauge transformation of the adiabatic phase:

$$\gamma_n(\mathcal{C}) \longrightarrow \gamma_n(\mathcal{C}) + \lambda_n(R_i^\mu) - \lambda_n(R_f^\mu)\,.$$

Therefore, if the path in parameter space $\mathcal{C}$ is closed (i.e., start and ends at the same place) then the adiabatic phase is a physical gauge-invariant quantity.

We can rewrite Berry's phase in a manifestly gauge-invariant forms if we introduce *Berry's curvature 2-form* as:

$$F_n(R^\mu) := \mathrm{d}A_n = \mathrm{i}\,\langle\partial_\mu n|\partial_\nu n\rangle\,\mathrm{d}R^\mu\wedge\mathrm{d}R^\nu\ , \tag{7}$$

where the term with double derivative $\partial_\mu\partial_\nu n$ has vanished because of the antisymmetry of the wedge product. It is easy to see that the exterior derivative identity $\mathrm{d}^2 = 0$ implies that Berry's curvature is gauge-invariant. If we can express the curve $\mathcal{C}$ as a boundary of a surface Σ, something that can be done if the topology of the parameter space is simple enough, then we can use Stokes theorem to express the integral over the boundary as an integral over the surface: $\int_{\partial\Sigma} A_n = \int_\Sigma \mathrm{d}A_n$. Consequently, we can express Berry's phase as:

$$\gamma_n(\mathcal{C}) := \oint_{\mathcal{C}} A_n = \int_\Sigma F_n\,. \tag{8}$$

B. Mead-Truhlar's curvature formula

We can find an alternative expression to (7) for Berry's curvature by utilizing the equation (3), with time derivatives $\mathrm{d}/\mathrm{d}t$ replaced by partial derivatives in parameter space $\partial_\mu = \partial/\partial R^\mu$:

$$\langle n|\partial_\mu k\rangle = \frac{\langle n|\partial_\mu\hat{H}|k\rangle}{E_k - E_n}\,.$$

First we write (7) by tacking the imaginary part, secondly we insert a resolution of the identity, thirdly we drop the $k = n$ term because it's real:

$$\begin{aligned} F_n &= -\operatorname{Im}\langle\partial_\mu n|\partial_\nu n\rangle\,\mathrm{d}R^\mu\wedge\mathrm{d}R^\nu \\ &= -\operatorname{Im}\sum_k \langle\partial_\mu n|k\rangle\,\langle k|\partial_\nu n\rangle\,\mathrm{d}R^\mu\wedge\mathrm{d}R^\nu \\ &= -\operatorname{Im}\sum_{k\neq n} \langle\partial_\mu n|k\rangle\,\langle k|\partial_\nu n\rangle\,\mathrm{d}R^\mu\wedge\mathrm{d}R^\nu\ , \end{aligned}$$

and lastly using the aforementioned relation for $\langle n|\partial_\mu k\rangle$ we get Mead-Truhlar's curvature formula:

$$F_n = -\sum_{k\neq n} \operatorname{Im}\frac{\langle n|\partial_\mu\hat{H}|k\rangle\langle k|\partial_\nu\hat{H}|n\rangle}{(E_n - E_k)^2}\,\mathrm{d}R^\mu\wedge\mathrm{d}R^\nu\ . \tag{9}$$

From this expression we see that Berry's curvature has singularities at points in parameter space where the Hamiltonian's spectrum has accidental degeneracies $E_{k\neq n} = E_n$. These singularities can make the parameter space topologically non-trivial and lead to interesting effects. For an example, for a topologically non-trivial parameter space, the adiabatic phase can be non-zero even if Berry's curvature is zero!

In the special case in which all energies of a given Hamiltonian are nondegenerate, we can prove that the following relation holds:

$$\sum_n F_n = 0\,, \tag{10}$$

where the sum n goes over the entire Hamiltonian spectrum. This equation follows from the differentiated orthonormalization conditions $\partial_\mu\langle n|m\rangle = \langle n|\partial_\mu m\rangle + \langle\partial_\mu n|m\rangle = 0$ that allow us to write F_n as:

$$F_n = \operatorname{Im}\sum_{k\neq n}\langle n|\partial_\mu k\rangle\,\langle k|\partial_\nu n\rangle\,\mathrm{d}R^\mu\wedge\mathrm{d}R^\nu\ ,$$

from which we see that the k-th term in the sum for F_n and the n-th term in the sum for F_k cancel each other out. This proves the relation.

Finally, we note that these two expressions that relate Berry's curvature to the rest of the Hamiltonian's spectrum somewhat obscure the origin of the adiabatic phase that according to equations (6) and (7) depends only on the respective eigenspace of the Hamiltonian. This will be important to keep in mind when we try to mathematically formalize and generalize Berry's phase.

Going forward, we would like to clarify a bit the terminology that we will use in the rest of the paper. A *phase* will loosely mean either a complex number of the form $\mathrm{e}^{\mathrm{i}x} \in \mathrm{U}(1)$ or a unitary matrix $U \in \mathrm{U}(N)$. The term *adiabatic phase* will refer to all non-dynamical phases that occur during adiabatic variation of the external parameters. In case the relevant eigenspace is nondegenerate, we shall also call this adiabatic phase *Berry's phase*, in case it's degenerate we shall call it *Wilczek-Zee's phase* (or unitary matrix). Other more general phases that are non-dynamical in nature we shall call *geometrical phases*,

an example being the Aharonov-Anandan phase. If the phase turns out to be insensitive to continuous variations of the path we shall call it a *topological phase*, an example of which will be given in the next section.

III. EXAMPLES

It is illustrative to study some simple examples of the Berry's phase in action. In this section we shall shortly analyse a spin $\frac{1}{2}$ and a spin s particle in a magnetic field, whose variation will lead to an adiabatic phase. We end this section by an application of the adiabatic phase to the Aharonov-Bohm effect.

A. Spin $\frac{1}{2}$ particle

The dynamics of a spin $\frac{1}{2}$ particle that is positioned in a magnetic field of strength $\mathbf{B}$ is governed by the Hamiltonian:

$$\hat{H}(\mathbf{B}) = -\hat{\boldsymbol{\mu}} \cdot \mathbf{B} = -\gamma \hat{\mathbf{S}} \cdot \mathbf{B}\,, \tag{11}$$

where $\hat{\boldsymbol{\mu}}$ is the magnetic moment of the particle, γ the gyromagnetic ratio of the particle, and $\hat{\mathbf{S}} = \frac{\hbar}{2}\boldsymbol{\sigma}$ the spin operator. If we use spherical coordinates ϑ and φ to describe the direction of the magnetic field, then we can express the eigenvector of the Hamiltonian as:

$$|+;\vartheta,\varphi\rangle = \begin{pmatrix} \cos\frac{\vartheta}{2} \\ \sin\frac{\vartheta}{2}\,\mathrm{e}^{\mathrm{i}\varphi} \end{pmatrix},$$
$$|-;\vartheta,\varphi\rangle = \begin{pmatrix} -\sin\frac{\vartheta}{2} \\ \cos\frac{\vartheta}{2}\,\mathrm{e}^{\mathrm{i}\varphi} \end{pmatrix}.$$

The corresponding energies are of course:

$$E_\pm = \mp\tfrac{1}{2}\gamma\hbar B\,.$$

Let us imagine a system that was initially in the $|+\rangle$ state, i.e., its spin was directed along the initial magnetic field. Moreover, let us imagine varying this magnetic field adiabatically afterwards. Then the state will acquire an adiabatic phase that is determine by Berry's connection 1-form and curvature 2-form. A little algebra using (6) and (7) shows that:

$$A_+(\vartheta,\varphi) = -\sin^2\tfrac{\vartheta}{2}\,\mathrm{d}\varphi\,,$$
$$F_+(\vartheta,\varphi) = -\tfrac{1}{2}\sin\vartheta\,\mathrm{d}\vartheta\wedge\mathrm{d}\varphi\,.$$

The expression for Berry's vector potential A_+ is not defined at the $\vartheta = \pi$ pole, reflecting the fact that our expression for $|+;\vartheta,\varphi\rangle$ is ill-defined at $\vartheta = \pi$. In particular, $|+;\pi,\varphi\rangle$ depends on φ, despite the fact that for all φ the coordinates $(\vartheta = \pi, \varphi)$ represent the same point on the 2-sphere. Furthermore, such a point where A_+ is undefined cannot be removed by a gauge transformation $A_+ \to A_+ + \mathrm{d}\lambda$, but only moved around the sphere. This reflects the non-triviality of this particular configuration of Berry's connection 1-form on the 2-sphere, something that we'll come back to later.

The fact that A_+ is undefined at the pole means that the calculated F_+ formally also isn't defined at the pole. Therefore, to calculate the value of F_+ for $\vartheta = \pi$ we should change to a different gauge where A_+ is defined at the pole, and then calculate F_+. Fortunately enough, in Berry's curvature we recognize the area 2-form $\mathrm{d}\Omega = \sin\vartheta\,\mathrm{d}\vartheta\wedge\mathrm{d}\varphi$ of the 2-sphere that we can safely analytically continue in to the formally undefined region. Hence, if the magnetic field direction unit vector traverses a certain closed path $\mathcal{C}$ on the unit 2-sphere, then the corresponding adiabatic phase given by (8) can be expressed using the solid angle $\Omega(\mathcal{C})$ that this path outlines:

$$\exp\{\mathrm{i}\gamma_+(\mathcal{C})\} = \exp\{-\tfrac{1}{2}\mathrm{i}\,\Omega(\mathcal{C})\}\,.$$

For the case of an initial $|-\rangle$ state, we use equation (10) do determine $F_- = -F_+$. Therefore, we have:

$$\exp\{\mathrm{i}\gamma_-(\mathcal{C})\} = \exp\{+\tfrac{1}{2}\mathrm{i}\,\Omega(\mathcal{C})\}\,.$$

A remarkable consequence of these two formulas is that slowly rotating a spin $\frac{1}{2}$ particle around the equator $\vartheta = \pi/2$ results in the wave function changing sign. This reflects the fact that the SU(2) group of rotation of spinors is a double cover of the SO(3) group of rotation of 3-vectors that we are accustomed to.

As it can be seen from the previous expressions, as we come closer and closer to the degeneracy point $\mathbf{B} = \mathbf{0}$, smaller and smaller variations of the magnetic field can achieve the same adiabatic phase as long as the subtended solid angles are the same. This is a consequence of the singularity of $F_\pm$ at the degeneracy point that can most easily be seen by switching from the spherical (B,ϑ,φ) to the Cartesian (B_1,B_2,B_3) coordinates:

$$F_\pm = \mp\frac{\epsilon_{ijk}}{4B^3}B_i\,\mathrm{d}B_j\wedge B_k\,,$$

where ϵ_{ijk} is the Levi-Civita symbol, and the indices i,j,k are to be summed over the range $1,2,3$. From the Mead-Truhlar formula (9) we expected this, and the $1/B^2$ character of the singularity can be traced down to the denominator $(E_+ - E_-)^2 \propto B^2$ of (9).

Using the Mead-Truhlar formula, we can show that such $1/r^2$ singularities near degeneracies are in fact generic. Let a general system described by $\hat{H}(R^\mu)$ have a two-fold degeneracy at $R^\mu = 0$ with the degenerate energies there being zero, $E_\pm(0) = 0$. Then according to the Mead-Truhlar formula (9) for small R^μ the contributions of the two near-degenerate states $|\pm\rangle$ dominate the sum, and thus the effective Hamiltonian reduces to a 2×2 Hermitian matrix that may be written as $\hat{H}(R^\mu) \simeq \mathbf{C}(R^\mu)\cdot\boldsymbol{\sigma}$. Since this Hamiltonian differs from the spin $\frac{1}{2}$ Hamiltonian (11) by a constant, we conclude that Berry's curvature 2-form has the same form just with the replacement $\mathbf{B} \to \pm\mathbf{C}(R^\mu)$. Consequently,

Berry's phase is determined by the solid angle that the vector $\mathbf{C}$ outlines. To come back to the original parameter space, we use $\mathrm{d}C_i = \partial_\mu C_i \,\mathrm{d}R^\mu$.

B. Spin s particle

A little more complicated example is that of a general spin s (integer or half-integer) particle. Let the magnetic field's direction again be specified by spherical coordinates ϑ and φ, a let the initial state be that of spin component along the magnetic field m where $m \in \{-s, -s+1, \ldots, s-1, s\}$. If we again vary the magnetic field adiabatically, the system stays in the corresponding state up to a phase. The Hamiltonian is the same as in the spin $\frac{1}{2}$ case, just with the spin $\frac{1}{2}$ operator exchanged by the general spin s operator $\hat{\mathbf{S}}$.

The energy of the m-th eigenstate is of course:

$$E_m = -m\gamma\hbar B\,.$$

To express the m-th eigenstate we need to rotate it away from the z-axis using Wigner's D-function:

$$|m;\vartheta,\varphi\rangle = \hat{D}(\varphi,\vartheta,-\varphi)\,|m\rangle_{\hat{\mathbf{z}}}\ ,$$

that is defined using the three dimensionless spin operators $(\hat{s}_x, \hat{s}_y, \hat{s}_z)$ and three Euler angles (α, β, γ) as:

$$\hat{D}(\alpha,\beta,\gamma) := \mathrm{e}^{-\mathrm{i}\alpha\hat{s}_z}\mathrm{e}^{-\mathrm{i}\beta\hat{s}_y}\mathrm{e}^{-\mathrm{i}\gamma\hat{s}_z}\ .$$

The angle $\gamma = -\varphi$ in the definition of $|m;\vartheta,\varphi\rangle$ has been chosen so that for $\vartheta = 0$ we have $|m;0,\varphi\rangle = |m\rangle_{\hat{\mathbf{z}}}$. The influence of this angle γ can be factored out, yielding:

$$|m;\vartheta,\varphi\rangle = \mathrm{e}^{im\varphi}\hat{D}(\varphi,\vartheta,0)\,|m\rangle_{\hat{\mathbf{z}}}\ .$$

To evaluate Berry's connection 1-form, we'll need to prove these two identities:

$$\hat{D}^\dagger(\varphi,\vartheta,0)\partial_\vartheta\hat{D}(\varphi,\vartheta,0) = -\mathrm{i}\hat{s}_y\,,\ \text{and}$$
$$\hat{D}^\dagger(\varphi,\vartheta,0)\partial_\varphi\hat{D}(\varphi,\vartheta,0) = -\mathrm{i}\cos\vartheta\,\hat{s}_z + \mathrm{i}\sin\vartheta\,\hat{s}_x\,.$$

The proof of the first ∂_ϑ identity is simply a straightforward differentiation of an exponential. To prove the second ∂_φ identity we first note that because of the commutation of operators $\hat{A}$ with their exponentials $\exp(\hat{A})$ we have:

$$\hat{D}^\dagger(\varphi,\vartheta,0)\partial_\varphi\hat{D}(\varphi,\vartheta,0) = \hat{D}^\dagger(0,\vartheta,0)(-\mathrm{i}\hat{s}_z)\hat{D}(0,\vartheta,0)\,,$$

which we can easily express using the fact that $\hat{\mathbf{s}}$ is a vector operator which satisfies:

$$\hat{D}^\dagger(\alpha,\beta,\gamma)\hat{s}_k\hat{D}(\alpha,\beta,\gamma) = R_{k\ell}(\alpha,\beta,\gamma)\hat{s}_\ell\,,$$

where $R_{k\ell}$ is the active 3-vector rotation matrix. In our particular case, the rotation of $\hat{s}_z$ by an angle ϑ around the y axis results in:

$$\hat{D}^\dagger(0,\vartheta,0)\hat{s}_z\hat{D}(0,\vartheta,0) = \cos\vartheta\,\hat{s}_z - \sin\vartheta\,\hat{s}_x\,,$$

from which the ∂_φ identity follows.

The Berry's connection 1-form and curvature 2-form can be calculated using equations (6) and (7), the previously proved ∂_ϑ and ∂_φ identities, and the fact that the spin operators $\hat{s}_x$ and $\hat{s}_y$ have vanishing diagonal matrix elements in the $|m\rangle_{\hat{\mathbf{z}}}$ basis:

$$A_m(\vartheta,\varphi) = m(\cos\vartheta - 1)\,\mathrm{d}\varphi\ ,$$
$$F_m(\vartheta,\varphi) = -m\sin\vartheta\,\mathrm{d}\vartheta\wedge\mathrm{d}\varphi\ .$$

The eigenvectors $|m;\vartheta,\varphi\rangle$ that we're using are again ill-define at the pole $\vartheta = \pi$, leading to the same problems as in the previous section. This time around, we'll be pedantic and use a gauge transformation $|m;\vartheta,\varphi\rangle \to \mathrm{e}^{-\mathrm{i}2m\varphi}\,|m;\vartheta,\varphi\rangle$ to find the vector potential $A'_m(\vartheta,\varphi) = m(\cos\vartheta+1)\,\mathrm{d}\varphi$ that is ill-defined only at the $\vartheta = 0$ pole. Both connection 1-forms result in the same curvature 2-form expression, for which we have now proved that it is valid across the entire 2-sphere. In this expression we again recognize the are area 2-form of the 2-sphere, thus implying:

$$\exp\{\mathrm{i}\gamma_m(\mathcal{C})\} = \exp\{-\mathrm{i}m\Omega(\mathcal{C})\}\,.$$

These results match with the results of the previous subsection. The relation (10) is also satisfied, as it should be.

C. Aharonov-Bohm effect

In their 1959 article Y. Aharonov and D. Bohm [3] studied how the existence of a non-zero magnetic vector potential can effect quantum particles even if the magnetic field is zero! This same effect we shall rederive here using Berry's phase.

Following Berry's original 1984 article [1], we consider a particle of charge q that is trapped in a box in which there is no magnetic vector potential, $\mathbf{A} = \mathbf{0}$. The box's position we shall describe with a 3-vector $\mathbf{R} \in \mathbb{R}^3$. Then the Hamiltonian of the system can be written as: $\hat{H} = H(\hat{\mathbf{p}}, \hat{\mathbf{r}} - \mathbf{R})$, and the wave functions of energy E_n are independent of $\mathbf{R}$ and have the form $\psi_n(\mathbf{r} - \mathbf{R})$. The wave function vanishes outside of the box.

If we now introduce a magnetic vector potential $\mathbf{A}$, but still presume the magnetic field to be zero, i.e., $\mathbf{B} = \boldsymbol{\nabla}\times\mathbf{A} = \mathbf{0}$ inside the box, then Hamiltonian minimally couples to it by way of:

$$H(\hat{\mathbf{p}} - q\mathbf{A}(\hat{\mathbf{r}}), \hat{\mathbf{r}} - \mathbf{R})\,|n,\mathbf{R}\rangle = E_n\,|n,\mathbf{R}\rangle\ ,$$

and this allows us to write down the corresponding wave function as:

$$\langle\mathbf{r}|n,\mathbf{R}\rangle = \exp\left\{\frac{\mathrm{i}q}{\hbar}\int_{\mathbf{R}}^{\mathbf{r}}\mathrm{d}\mathbf{r}'\cdot\mathbf{A}(\mathbf{r}')\right\}\psi_n(\mathbf{r}-\mathbf{R})\,.$$

This solution as defined above is well-define since it is single-valued inside the box, and it is single-valued because the box is simply connected and the curl of $\mathbf{A}$ vanishes making the integral in the exponential depend only upon the endpoints.

Now, if we imagine having an ideal solenoid positioned along the z-axis and adiabatically transporting this box around a closed path $\mathcal{C}$ outside of the solenoid, we shall get an adiabatic phase that after a little algebra using equations (6) and (8) turns out to be:

$$\gamma_n(\mathcal{C}) = \frac{q}{\hbar}\oint_{\mathcal{C}} \mathrm{d}\mathbf{R}\cdot\mathbf{A}(\mathbf{R}) = \frac{q\Phi_B}{\hbar}\cdot w(\mathcal{C})\,,$$

where Φ_B is the magnetic flux of the solenoid and $w(\mathcal{C})$ the winding number of the path around the solenoid. Thus, we see that the Berry's connection 1-form, that we suggestively called Berry's vector potential, now becomes directly proportional to the magnetic vector potential of electrodynamics. This expression for Berry's phase is equal to the phase that Aharonov and Bohm originally derived. Another special feature of this phase is that it depends only on the *topology* of the path, which in this case means the winding number. Such phases, when they occur, we shall call *topological phases*, and the main thing that distinguishes them from more general geometric phases is that they are insensitive to the details of the shape of the path.

IV. WILCZEK-ZEE'S PHASE

Up until now we have limited ourselves to studying the geometric phase that accompanies the adiabatic evolution of *nondegenerate* eigenstate. In this section we remove this assumption and study the adiabatic evolution of a system that was initially an element of a degenerate eigenspace. As we shall see, the Berry's phase of the nondegenerate case will generalize to the Wilczek-Zee's unitary matrix of the degenerate case.

Suppose that the n-th eigenvalues of the Hamiltonian is M-times degenerate across the entire parameter space, as in:

$$\hat{H}(R^\mu)\,|n,a,R^\mu\rangle = E_n(R^\mu)\,|n,a,R^\mu\rangle\ , \tag{12}$$

with $a = 1,2,\ldots,M$. Going forward, indices $a,b,c,\ldots$ will be summed over $1,2,\ldots,M$ by the Einstein's summation convention, and the index n will be dropped from all the kets. Then we may choose the eigenstates to be an orthonormal basis of the underlying eigenspace, i.e., $\langle a|b\rangle = \delta_{ab}$. Clearly, there is a $\mathrm{U}(M)$ gauge freedom in doing so, for we can always redefine the basis vector according to:

$$|a,R^\mu\rangle \longrightarrow \Omega_{ab}(R^\mu)\,|b,R^\mu\rangle\ , \tag{13}$$

where $\Omega_{ab}(R^\mu) \in \mathrm{U}(M)$ is a smooth unitary matrix-valued function of the external parameters.

Let us consider a system whose state $|\psi(t)\rangle$ was initially in the n-th degenerate subspace. In the adiabatic limit, as we vary the external parameters, the state will stay in the degenerate subspace, and we may write it as:

$$|\psi(t)\rangle = \mathrm{e}^{i\vartheta_n(t)}\psi_a U^{(n)}_{ab}(t)\,|b,R^\mu(t)\rangle\ ,$$

where ϑ_n is the dynamical phase, $\psi_a = \langle a|\psi(0)\rangle$ the initial state coefficients, and $U^{(n)}_{ab}$ the *Wilczek-Zee's unitary matrix*. By substituting this Ansatz in to the Schrödinger equation (2), acting from the left by $\langle c|$, and rearranging, we get the equations of motion for the Wilczek-Zee's phase:

$$\dot{U}^{(n)}_{ac}(t) = -\,\langle c|\frac{\mathrm{d}}{\mathrm{d}t}|b\rangle\,U^{(n)}_{ab}(t)\,,\ \text{or}$$
$$\left(U^\dagger\dot{U}\right)^{(n)}_{ab} = -\,\langle b|\frac{\mathrm{d}}{\mathrm{d}t}|a\rangle\ .$$

The initial conditions are $\dot{U}^{(n)}_{ab}(0) = \delta_{ab}$.

The equations of motion naturally lead us towards defining the *Wilczek-Zee's curvature 1-form*:

$$A^{(n)}_{ab} := \mathrm{i}\,\langle b|\mathrm{d}a\rangle = \mathrm{i}\,\langle b|\partial_\mu a\rangle\,\mathrm{d}R^\mu\ , \tag{14}$$

that we interpret as a Hermitian matrix-valued 1-form in parameter space. (The hermicity follows from the orthonormalization condition $\langle a|b\rangle = \delta_{ab}$.) Using the equations of motion, we can explicitly express the Wilczek-Zee's unitary matrix as a Dyson series, i.e., a path-ordered exponential integral:

$$U^{(n)}(\mathcal{C}) := \mathcal{P}\exp\left(\mathrm{i}\int_{\mathcal{C}} A^{(n)}\right)\ , \tag{15}$$

Here, $\mathcal{P}$ is the path-ordering operator, and the integral is over the oriented path $\mathcal{C}$ in parameter space, formerly described by $R^\mu(t)$. Clearly, this expression reduces to the familiar Berry's phase in the nondegenerate $M = 1$ case. Finally, we can also define a generalization of the Berry's curvature 2-form, the *Wilczek-Zee's curvature 2-form*, as:

$$F^{(n)} := \mathrm{d}A^{(n)} + \mathrm{i}A^{(n)}\wedge A^{(n)}\,,\ \text{or}$$
$$F^{(n)}_{\mu\nu} = \partial_\mu A^{(n)}_\nu - \partial_\nu A^{(n)}_\mu + \mathrm{i}\left[A^{(n)}_\mu, A^{(n)}_\nu\right]\ . \tag{16}$$

This Wilczek-Zee's curvature is a Hermitian matrix-valued 2-form in parameter space. If we furthermore want to express the Wilczek-Zee's phase as an area integral using this curvature 2-form, we would have to use the non-abelian Stokes theorem. Although we shall not pursue this matter here, we will note that Wilczek-Zee's phase cannot be expressed solely in terms of $F^{(n)}$.

Lastly, we study how all of these introduced object change after a $\mathrm{U}(M)$ gauge transformation described by (13). We start with the connection 1-form $A^{(n)}$. After substituting equation (13) in to the definition (14), and rearranging we obtain:

$$A^{(n)} \longrightarrow \Omega A^{(n)}\Omega^\dagger + \mathrm{i}\,\mathrm{d}\Omega\,\Omega^\dagger\,,$$

where $\mathrm{d}\Omega = \partial_\mu\Omega\,\mathrm{d}R^\mu$. For the curvature 2-form a similar calculation leads us towards the following gauge covariant transformation:

$$F^{(n)} \longrightarrow \Omega F^{(n)}\Omega^\dagger\,.$$

For the Wilczek-Zee's unitary matrix we use the fact that the physical state $|\psi(t)\rangle$ is independent of the eigenspace basis that we use to express it, i.e.,

$$\mathrm{e}^{-\mathrm{i}\vartheta_n(t)}\,|\psi(t)\rangle = \psi'_a U^{(n)\prime}_{ab}(t)\,|b'\rangle = \psi_a U^{(n)}_{ab}(t)\,|b\rangle\ .$$

After some algebraic manipulations we derive the following transformation law for Wilczek-Zee's phase:

$$U^{(n)} \longrightarrow \Omega(R^\mu_i)U^{(n)}(\mathcal{C})\Omega^\dagger(R^\mu_f)\,.$$

In the case of a nondegenerate $M = 1$ eigenspace, all these transformation laws reduce to the ones we derived earlier for Berry's connection, curvature and phase.

In the case that the path $\mathcal{C}$ is closed, Wilczek-Zee's phase transforms as a matrix under a change of basis. Thus, although Wilczek-Zee's phase is not a gauge-invariant quantity, its coefficients of the characteristic polynomial and eigenvalues are. One matrix-invariant that is often used in this context is the *Wilson loop* that is defined as:

$$W^{(n)}(\mathcal{C}) := \mathrm{tr}\,U^{(n)}(\mathcal{C}) = \mathrm{tr}\left\{\mathcal{P}\exp\left(\mathrm{i}\oint_{\mathcal{C}} A^{(n)}\right)\right\}\ .$$

And with that we have finished the formalism of non-degenerate adiabatic evolution. As one can see, it is significantly more complicated owning to the fact that the gauge group $\mathrm{U}(M)$ is non-abelian. Fortuitously, all of this formalism occurs in other branches of physics – most notably in Yang-Mills gauge theory, and as such it's probably familiar to a big portion of the readership.

After this we could cook up some simple examples just to see this formalism in action, but we shall rather favor discussing a more interesting real-world example that shares the same mathematical structure – that of molecular dynamics. For the readers that would like to see some simple examples analysed, we direct them towards chapter 2, section 3 of [21].

V. THE GAUGE THEORY OF MOLECULAR PHYSICS

In the analysis of complicated physical systems made of many particles that we want to fully treat quantum mechanically (so we can't just average out a part, treat it classically, or consider it imposed externally by the environment), our most reliable method is to *separate* the system in to simpler subsystems and analyse them separately. Afterwards, we combine the analyses to get a complete picture. A natural separation of that sort is the separation of the system in to *fast* and *slow* moving degrees of freedom (DOF), the paradigmatic example being the Born-Oppenheimer method of molecular physics.

In the conventional Born-Oppenheimer approximation, the molecule is separated in to the fast electronic and slow nuclear DOFs. First, the electronic energies and wave functions are calculated whilst keeping the positions of the ions fixed. Then some approximations are used to get the effective Hamiltonian of the ions, given an electronic configuration. Using this Hamiltonian, the wave functions of the ions are calculated. Finally, the results are combined to give the total wave function.

It turns out that the original approximations that were used for getting the effective ionic Hamiltonian are too crude to capture important effects that owe their origin to the geometrical potential and phase. A more complete adiabatic approximation naturally leads to a molecular gauge theory that incorporates these geometric effects. Historically, the importance of these geometric effects was first recognized in vibronic (vibrational and electronic) problems in Jahn-Teller systems where certain sign-changes could not be accounted for.

The starting point of analysing molecules is the Hamiltonian, that for our purposes is made of the non-relativistic kinetic energies of the electrons and nuclei, and the instantaneous Coulomb potential of electrons and nuclei among themselves and between each other. The number of electrons is N_e, and the number of nuclei is N_n. There are in total $3N_e + 3N_n$ space DOFs – three of which are centre of mass (CM) translation and three orientation (rotation) of the molecule. Spin degrees of freedom will not be important in our analysis, except for the quantum statistics that they entail.

In the usual analysis of molecules both translational and rotational DOFs of the molecule as a whole are isolated by a change of coordinates, but such procedures lead to very complicated kinetic terms and as such aren't convenient for our analysis. To simplify the kinetic energy operator of the nuclei (that generally have different masses) and remove the center of mass contribution to the kinetic energy, Jacobi's coordinates are used to describe the positions of nuclei. Jaobi's coordinates are shortly described in the appendix A. The final result of this change of coordinates is that the total internal (as in no CM terms) Hamiltonian of the systems becomes:

$$\hat{H} = \frac{\hat{\mathbf{P}}^2}{2\mu} + h(\hat{\mathbf{p}}, \hat{\mathbf{R}}, \hat{\mathbf{r}})\,, \tag{17}$$

where h is the electronic part of the Hamiltonian:

$$h(\hat{\mathbf{p}}, \hat{\mathbf{R}}, \hat{\mathbf{r}}) = \frac{\hat{\mathbf{p}}^2}{2m_e} + V(\hat{\mathbf{R}}, \hat{\mathbf{r}})\,. \tag{18}$$

The operators $\hat{\mathbf{R}}$ and $\hat{\mathbf{P}}$ are $(3N_n - 3)$ dimensional nuclear position and momentum operators in Jacobi's coordinates, while the operators $\hat{\mathbf{r}} = (\hat{\mathbf{r}}_1, \cdots, \hat{\mathbf{r}}_{N_e})$ and $\hat{\mathbf{p}} = (\hat{\mathbf{p}}_1, \cdots, \hat{\mathbf{p}}_{N_e})$ are the $3N_e$ dimensional electronic position and momentum operators in their usual Cartesian coordinates, with the individual electrons coordinates concatenated for convenience. The potential $V(\hat{\mathbf{R}}, \hat{\mathbf{r}})$ includes all other terms that depend only on $\hat{\mathbf{R}}$ and $\hat{\mathbf{r}}$, in this case the electron, nuclear and electron-nuclear Coulomb potential.

Now we split the system in to two parts, the fast or electronic part described by $\hat{\mathbf{r}}$ and $\hat{\mathbf{p}}$, and slow or nuclear

part described by $\hat{\mathbf{R}}$ and $\hat{\mathbf{P}}$. The total state space we may write as a direct product $\mathcal{H} = \mathcal{H}^{\text{slow}} \otimes \mathcal{H}^{\text{fast}}$, and for a basis of the total state space it is convenient to use the kets $|\mathbf{R}, n\rangle$ that are defined by:

$$\hat{\mathbf{R}} \, |\mathbf{R}, n\rangle \doteq \mathbf{R} \, |\mathbf{R}, n\rangle \ ,$$
$$h(\hat{\mathbf{p}}, \hat{\mathbf{R}}, \hat{\mathbf{r}}) \, |\mathbf{R}, n\rangle \doteq \epsilon_n(\mathbf{R}) \, |\mathbf{R}, n\rangle \ .$$

This can be done since $[\hat{\mathbf{R}}, \hat{h}] = 0$. We may also write these kets as a pseudo-direct product $|\mathbf{R}\rangle \tilde{\otimes} |n(\mathbf{R})\rangle$, pseudo because the quantum numbers $\mathbf{R}$ and n are not independent and as such do not define vector subspaces. If we want to go back to the $|\mathbf{R}, \mathbf{r}\rangle$ basis, we use:

$$\langle \mathbf{R}', \mathbf{r}' | \mathbf{R}, n \rangle = \delta^{3N_n - 3}(\mathbf{R}' - \mathbf{R}) \, \langle \mathbf{r}' | n(\mathbf{R}) \rangle \ .$$

Here comes the most important part of the analysis. Because of the interdependence of eigenstates $|n(\mathbf{R})\rangle$ on $\mathbf{R}$, when we expand the action of the momentum operator $\hat{\mathbf{P}}$ in the $|\mathbf{R}, n\rangle$ basis we get an additional term (beside the usual $-\mathrm{i}\hbar\boldsymbol{\nabla}$) – *the Mead gauge potential*. In particular, we may write:

$$\langle \mathbf{R}, n | \hat{\mathbf{P}} | \psi \rangle = \sum_m -\mathrm{i}\hbar \mathbf{D}^{nm} \, \langle \mathbf{R}, m | \psi \rangle \ ,$$

where $\mathbf{D}^{nm}$ is the covariant derivative:

$$\mathbf{D}^{nm} := \boldsymbol{\nabla}_{\mathbf{R}} \delta^{nm} - \mathrm{i}\mathbf{A}^{nm}(\mathbf{R}) \, , \tag{19}$$

and $\mathbf{A}^{nm}$ is the Mead gauge potential:

$$\mathbf{A}^{nm}(\mathbf{R}) := \mathrm{i} \, \langle n(\mathbf{R}) | \boldsymbol{\nabla}_{\mathbf{R}} | m(\mathbf{R}) \rangle \ . \tag{20}$$

The derivation of this result is straightforward but lengthy, so we refer the readers towards chapter 8, section 3 of [20]. With this exact result we can reformulate the problem of diagonalizing the Hamiltonian (17).

Let $\left|\psi^E\right\rangle$ be the total state of the system with total energy E:

$$\hat{H} \left|\psi^E\right\rangle = E \left|\psi^E\right\rangle \ ,$$

and $\psi^E(\mathbf{R}, \mathbf{r}) = \left\langle \mathbf{R}, \mathbf{r} \middle| \psi^E \right\rangle$ its wave function. Then, conventionally, we find the energy E and wave function $\psi^E(\mathbf{R}, \mathbf{r})$ by solving the stationary Schrödinger equation – a partial differential equation in the variables $\mathbf{R}$ and $\mathbf{r}$. Instead of this, what we'll do here is decompose this problem in to two parts. For that, we first introduce two auxiliary wave functions:

$$\psi_n^E(\mathbf{R}, \mathbf{r}) := \left\langle \mathbf{R}, n \middle| \psi^E \right\rangle \ ,$$
$$\varphi_n(\mathbf{R}, \mathbf{r}) := \langle \mathbf{r} | n(\mathbf{R}) \rangle \ ,$$

using which we can express the total wave function as:

$$\psi_n^E(\mathbf{R}, \mathbf{r}) = \sum_n \varphi_n(\mathbf{R}, \mathbf{r}) \psi_n^E(\mathbf{R}) \, .$$

Now we reformulate the problem. The first task is to solve the differential equation for the electronic wave functions keeping the positions of the ions fixed:

$$\left[\frac{-\hbar^2}{2m_e} \boldsymbol{\nabla}_{\mathbf{r}}^2 + V(\mathbf{R}, \mathbf{r}) \right] \varphi_n(\mathbf{R}, \mathbf{r}) = \epsilon_n(\mathbf{R}) \varphi_n(\mathbf{R}, \mathbf{r}) \, . \tag{21}$$

The second task is to solve the infinite number of coupled differential equations that determine the total wave function:

$$\sum_m \left[\frac{-\hbar^2}{2\mu} \sum_\ell \mathbf{D}^{n\ell} \mathbf{D}^{\ell m} + \epsilon_n(\mathbf{R}) \delta^{nm} \right] \psi_m^E(\mathbf{R}) = E \psi_n^E(\mathbf{R}) \, . \tag{22}$$

This procedure of diagonalizing the total Hamiltonian $\hat{H}$ is *exact*, if we have solved equation (21) exactly for all possible $\mathbf{R}$ and n. In practice, however, it is typically sufficient to consider only the lowest few $n = 1, 2, \ldots, \mathcal{N}$ electronic configurations and solve equation (21) only close to the equilibrium positions of $\mathbf{R}$. By restricting the indices n, m and ℓ of equation (22) to the range $1, \ldots, \mathcal{N}$ we get the *Born-Huang approximation* [22]. In contrast, in the Born-Oppenheimer approximation the equation (22) is taken to be:

$$\left[\frac{-\hbar^2}{2\mu} \boldsymbol{\nabla}_{\mathbf{R}}^2 + \epsilon_n(\mathbf{R}) \right] \psi_n^E(\mathbf{R}) = E \psi_n^E(\mathbf{R}) \, ,$$

and such disregards all geometric effect that owe their origin to the geometric Mead gauge potential defined in (20). In the Born-Huang approximation we have a natural gauge transformation that is determined by the degeneracies in the electronic spectrum of the $\mathcal{N}$-dimensional subspace that we limited ourselves to. In the case of no degeneracies, the gauge group is $\mathrm{U}(1)^{\mathcal{N}}$, in the case of an $\mathcal{N}$-fold degeneracy the gauge group is $\mathrm{U}(\mathcal{N})$, and in general it's something in between.

Up until now we have shown how an exact treatment of molecular dynamics leads us naturally towards introducing a gauge potential, covariant derivative, and other elements of a gauge theory. We shall finish this section not by introducing the whole formalism of molecular gauge theory, but rather by discussing some interesting physical implications of these geometric terms that we have found.

One interesting implication of molecular gauge theory is the generic appearance of effective magnetic monopole fields. In particular, whenever you have rapid rotation of the fast subsystem around the axis connecting two pieces of the slow subsystem, a monopole vector potential appears in the dynamics of the slow system.

Another interesting implication is how the existence of conical intersections (points in $\mathbf{R}$-space where the derivatives of $|n(\mathbf{R})\rangle$ are not well defined) causes the electronic wave functions $\varphi(\mathbf{R}, \mathbf{r})$ to change sign when they are transported around the conical intersection, thus making the electronic wave functions multi-valued in $\mathbf{R}$-space. This sign-changing behavior modifies the boundary conditions of the nuclear wave functions $\psi_n^E(\mathbf{R})$. Moreover,

the amplitude of the nuclear wave functions at the conical intersections vanishes because of the vibronic centrifugal (or Born-Huang) term. There is also a trade-off between choosing the electronic eigenvectors to be single-valued and making the Mead gauge potential vanish. In case we chose to make the electronic eigenvectors single-valued, these conical intersection points behave like magnetic flux sources. It's also interesting to note that even when the geometric curvature $\mathbf{F} = \mathrm{i}[\mathbf{D}, \mathbf{D}]$ derived from the covariant derivative (19) vanishes, there may still appear nontrivial geometric and topological effects analogous to the Aharonov-Bohm effect with conical intersections playing the role of the solenoid.

VI. AHARONOV-ANANDAN'S PHASE

In this section we generalize the notion of geometric phases from systems that evolve adiabatically to general systems that evolve cyclically. Berry's phase then arises as the adiabatic limit of this more general geometric phase.

Since the phase of a state vector in isolation is nonphysical, we introduce the *quantum phase space* or *projective Hilbert space* as the quotient space:

$$\mathcal{P}(\mathcal{H}) := \mathcal{S}(\mathcal{H})/\sim ,$$

where $\mathcal{H}$ is the Hilbert space of states, $\mathcal{S}(\mathcal{H})$ the sphere of all normalized vectors in $\mathcal{H}$, and the equivalence relation between vectors is defined as $|\phi\rangle \sim |\psi\rangle$ iff there exists a $\mathrm{e}^{\mathrm{i}\varphi} \in \mathrm{U}(1)$ such that $|\phi\rangle = \mathrm{e}^{\mathrm{i}\varphi}|\psi\rangle$. A ray $[|\psi\rangle]$ is by definition an element of the projective Hilbert space $\mathcal{P}(\mathcal{H})$, i.e., an equivalence class of vectors differing from the normalized state vector $|\psi\rangle$ by a phase. The ray of a normalized state of the system $|\psi\rangle$ can be conveniently represented by the unique projector $\hat{P}_\psi = |\psi\rangle\langle\psi|$.

For a system we say that it evolves cyclically when the rays corresponding to the initial and final state coincide. Thus, an evolution of the system $|\psi(t)\rangle$ during the time interval $t \in [0, T]$ is cyclic iff $\hat{P}_{\psi(0)} = \hat{P}_{\psi(T)}$, which is equivalent to the condition that $|\psi(T)\rangle = \mathrm{e}^{\mathrm{i}\varphi}|\psi(0)\rangle$ for some phase $\varphi \in \mathbb{R}$. Alternatively, an evolution of the state vector of the system becomes a curve in the projective Hilbert space, and we say that the evolution is cyclic iff the corresponding curve in $\mathcal{P}(\mathcal{H})$ is closed.

Consider a system described by the state vector $|\psi(t)\rangle$ that during the time interval $t \in [0, T]$ evolves cyclically with a total phase $\varphi \in \mathbb{R}$, i.e.,

$$|\psi(T)\rangle = \mathrm{e}^{\mathrm{i}\varphi}|\psi(0)\rangle .$$

The oriented path that the ray $P_{\psi(t)}$ traces in the quantum phase space $\mathcal{P}(\mathcal{H})$ during the time $[0, T]$ we shall denote as $\mathcal{C}$. Let the evolution of the system be describe by the Hamiltonian $\hat{H}(t)$, that in general has some time dependence. Then the evolution of the system is given either by the Schrödinger equation:

$$\mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t}|\psi(t)\rangle = \hat{H}(t)|\psi(t)\rangle , \tag{23}$$

or by the von Neumann equation:

$$\mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t}\hat{P}_{\psi(t)} = \left[\hat{H}(t), \hat{P}_{\psi(t)}\right] . \tag{24}$$

What we shall prove is that the phase φ can naturally be divided in to two parts: the dynamical phase φ_{dyn} that depends on the Hamiltonian and the geometrical phase φ_{AA} that depends only on the curve $\mathcal{C}$ in $\mathcal{P}(\mathcal{H})$.

To prove this, we note that the transformation of the Hamiltonian $\hat{H}(t) \to \hat{H}(t) + \mathbb{1}a(t)$ does not influence the path $\mathcal{C}$ in the quantum phase space $\mathcal{P}(\mathcal{H})$, since the von Neumann equation (24) is left unaffected. The solution to the Schrödinger equation, however, is effected:

$$|\psi(t)\rangle \longrightarrow |\psi'(t)\rangle = \exp\left\{-\frac{\mathrm{i}}{\hbar}\int_0^t \mathrm{d}t'\, a(t')\right\}|\psi(t)\rangle ,$$

and the total phase as well:

$$\varphi \longrightarrow \varphi' = \varphi - \frac{\mathrm{i}}{\hbar}\int_0^T \mathrm{d}t\, a(t) .$$

To find the geometric part of the phase, we choose the $\tilde{a}(t)$ in such a way that the $\tilde{\varphi} = 0$, so that the transformed state vector is periodic: $|\tilde{\psi}(T)\rangle = |\tilde{\psi}(0)\rangle$. This means that the path in $\mathcal{S}(\mathcal{H})$ traced by $|\tilde{\psi}(t)\rangle$ is closed. (We'll use tildes to mark quantities that are related to periodic state vectors.) Hence:

$$\varphi = \frac{\mathrm{i}}{\hbar}\int_0^T \mathrm{d}t\, \tilde{a}(t) .$$

By acting from the left by $\langle\tilde{\psi}(t)|$ on the new Schrödinger equation:

$$\mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t}|\tilde{\psi}(t)\rangle = \left(\hat{H}(t) + \mathbb{1}\tilde{a}(t)\right)|\tilde{\psi}(t)\rangle ,$$

and integrating from $t = 0$ to T, we get the desired equation for the total phase:

$$\begin{aligned} \varphi &= \varphi_{\mathrm{dyn}} + \varphi_{\mathrm{AA}} , \text{ where} \\ \varphi_{\mathrm{dyn}} &:= -\frac{1}{\hbar}\int_0^T \mathrm{d}t\ \langle\psi(t)|\hat{H}(t)|\psi(t)\rangle , \\ \varphi_{\mathrm{AA}} &:= \int_0^T \mathrm{d}t\, \mathrm{i}\,\langle\tilde{\psi}(t)|\frac{\mathrm{d}}{\mathrm{d}t}|\tilde{\psi}(t)\rangle . \end{aligned} \tag{25}$$

The phase φ_{AA} is the *Aharonov-Anandan's phase*.

We see from the expression for φ_{dyn} that the dynamical phase manifestly depends on the Hamiltonian of the system. On the other hand, if we are given a closed curve $\mathcal{C}$ in $\mathcal{P}(\mathcal{H})$ and take any state vector $|\tilde{\psi}(t)\rangle$ that is periodic and projects to the curve $\mathcal{C}$, we get the same value for φ_{AA}. To prove this, let us take another state vector $|\tilde{\psi}'(t)\rangle = e^{\mathrm{i}\lambda(t)}|\tilde{\psi}(t)\rangle$ with $\lambda(T) = \lambda(0)$. Then a simple calculation using (25) shows that:

$$\varphi'_{\mathrm{AA}} = \varphi_{\mathrm{AA}} + \lambda(0) - \lambda(T) = \varphi_{\mathrm{AA}} .$$

Not only is the expression for Aharonov-Anandan's phase independent of the choice of $|\tilde{\psi}(t)\rangle$, but it's also independent of the parameterization of $|\tilde{\psi}(t)\rangle$. This will lead us towards defining a connection 1-form on the quantum phase space $\mathcal{P}(\mathcal{H})$, much in the same way we introduce Berry's connection 1-form for adiabatic evolution. Since the quantum phase space is, in general, an infinite-dimensional manifold, this will be mathematically more demanding, and we defer the discussion of this to after we introduce the proper mathematical formalism. Here we just note that formally we can write the Aharonov-Anandan's phase as:

$$\varphi_{\mathrm{AA}} = \oint_{\mathcal{C}} \mathrm{i}\, \langle \tilde{\psi} | \mathrm{d}\tilde{\psi} \rangle \ .$$

Aharonov-Anandan's phase includes Berry's phase as a special case. To see how, we note that the adiabatic theorem implies that in the adiabatic limit the state vector will stay in the corresponding eigenspace $|n, R^{\mu}\rangle$ up to a phase. Therefore, to connect the results of this section with the result of our discussion of Berry's phase, we can simply substitute $|\tilde{\psi}(t)\rangle = |n, R^{\mu}(t)\rangle$.

VII. MATHEMATICAL FORMALISM

The mathematically inclined read may have noticed that the previous discussion of Berry's and Wilczek-Zee's phase implicitly uses many concepts from differential geometry: that of a vector bundle, principal U(N)-bundle, connection, horizontal lift, parallel transport, curvature 2-form and holonomy. In this section we shall incorporate these mathematical concepts in to a mathematical formalism of geometric phases. From the reader we expect familiarity with the basics of differential geometry: manifolds, tangent bundles, tensors, differential forms. Familiarity with vector bundles and connections on vector bundles (expressed using covariant derivatives) is useful bun not necessary. Other less-common knowledge we shall introduce here [23]. In the appendix we give a short review of Lie groups, Lie group actions and fibre bundles. Here, we introduce the two most important concepts – the principal bundle and Ehresmann connection.

A. Fibre G-bundles and principal G-bundles

All the manifolds and bundles of this section will be smooth, unless stated otherwise. A fibre bundle made of a total space E, base space B, projection π and fibre F we shall demarcate as $E(\pi, B, F)$, and the fibre over a point $x \in B$ we shall mark as $E_x = \pi^{-1}(x)$. Given two local trivialization $(U_\alpha \subseteq B, \varphi_\alpha \colon \pi^{-1}(U_\alpha) \to U_\alpha \times F)$ and (U_β, φ_β) the transition function we define as $\chi_{\alpha\beta}(x) := \varphi_\alpha \circ \varphi_\beta^{-1}|_x$. For a point $x \in U_\alpha \cap U_\beta$ the transition function $\chi_{\alpha\beta}(x)$ is a diffeomorphism of $\{x\} \times F \cong F$, i.e., $\chi_{\alpha\beta}(x) \in \mathrm{Diff}(F)$.

If the fibre F has some additional structure that we want to be preserved as we transition from one local trivialization to another, then we need to restrict the transition function to be elements of only a subset of $\mathrm{Diff}(F)$. We accomplish this by introducing a structure Lie group G together with a left group action $\Phi \colon G \times F \to F$, and then demanding that every transition function can be written as $\chi_{\alpha\beta}(x) = \Phi_g$ for some $g \in G$. This naturally leads us towards the definition of a fibre G-bundle.

A fibre G-bundle $E(\pi, B, F, G, \Phi)$ is a fibre bundle $E(\pi, B, F)$ together with a structure Lie group G which acts faithfully on F through a smooth left action $\Phi \colon G \times F \to F$. Furthermore, we demand that for every transition functions $\chi_{\alpha\beta}$ between two local trivializations $(U_\alpha, \varphi_\alpha)$ and (U_β, φ_β) there exists a smooth function $g_{\alpha\beta} \colon U_\alpha \cap U_\beta \to G$ that allows us to write $\chi_{\alpha\beta}(x) = \Phi_{g_{\alpha\beta}(x)}$. Among the various fibre G-bundles that one may define given a fixed base space B and structure group G, one of them stands out – the principal G-bundle.

A principal G-bundle $P(\pi, B, G)$ is a fibre G-bundle $P(\pi, B, F = G, G, \Phi = L)$ whose fibre coincides with the structure group G and whose left group action is simply the left translation $\Phi(g, h) = L(g, h) = L_g(h) = g \cdot h$. For convenience we may define the multiplication of $g \in G$ with an order pair $(x, h) \in B \times G$ as $g \cdot (x, h) = (x, g \cdot h)$ or $(x, h) \cdot g = (x, h \cdot g)$. Thus, if we have two local trivializations $(U_\alpha, \varphi_\alpha)$ and (U_β, φ_β), for a point $p \in P_x$ placed above $x = \pi(p) \in U_\alpha \cap U_\beta$, we may write:

$$\varphi_\alpha(p) = g_{\alpha\beta}(x) \cdot \varphi_\beta(p) \, .$$

Furthermore, we can naturally define a right group action on the total space $\tilde{R} \colon G \times P \to P$ by:

$$\tilde{R}(g, p) = \tilde{R}_g(p) = p \cdot g := \varphi_\alpha^{-1}(\varphi_\alpha(p) \cdot g) \, . \tag{26}$$

A simple calculation shows that this right action, as defined above, does not depend on the trivialization used to define it. This canonical right action is smooth, free and leaves the individual fibres invariant, i.e., $\pi(p) = \pi(p \cdot g)$ for all $g \in G$ and $p \in P$. Additionally, this right action restricted to one fibre acts transitively and freely upon it. Consequently, the orbit of a point $p \in E$ above $x = \pi(p)$ is equal to the fibre that it's an element of, i.e., $\mathrm{Orb}(p) = P_x$. (A short review of Lie group actions is given in appendix C.) The structure group G of the principal fibre bundle in the context of gauge theories is called the gauge or symmetry group.

To every fibre G-bundle $E(\pi, B, F, G, \Phi)$ we can associate a unique principal G-bundle $\hat{P}(\hat{\pi}, B, G)$. We do this by replacing the fibres E_x of E with copies of G and then gluing them together using the same transition function as in E. Explicitly, let $\{(U_\alpha, \varphi_\alpha)\}$ be a complete set of local trivializations of E, $\{\chi_{\alpha\beta}\}$ the transition functions among these local trivializations, and $\{g_{\alpha\beta}\}$ their matching group elements. Then we can construct the total space of the principal bundle as the quotient space:

$$\hat{P} = \bigsqcup_\alpha U_\alpha \times G / \sim \, ,$$

where the equivalence relation $\sim$ is defined by $(x,g)_\alpha \sim (y,h)_\beta$ iff $x = y$ and $g = g_{\alpha\beta}(x) \cdot h$. The projection we define in the obvious way as $\hat{\pi}((x,g)_\alpha) = x$; it is easy to see that the projection does not depend on the choice of the representative from the equivalence class $[(x,g)_\alpha]$. The principal G-bundle constructed in this way we call the *associated principal bundle* to the fibre G-bundle.

In the specific case in which the fibre G-bundle is a vector bundle (i.e., $F = k^N$ with $k = \mathbb{R}$ or $\mathbb{C}$ is a vector space and the structure group G is a subgroup of the general linear group $\mathrm{GL}(N,k)$) our previous construction gets an intuitive interpretation. The choice of a local trivialization $(U_\alpha, \varphi_\alpha)$ on this vector bundle amounts to choosing which local basis to use for expressing vectors of E_x, where $x \in U_\alpha$. An element $p \in \hat{P}$ with $x = \hat{\pi}(p)$ can be interpreted as a particular choice of a *frame* or *ordered basis* of the fiber E_x, where the vectors of the frame are the columns of the corresponding $\mathrm{GL}(N,k)$ matrix. In particular, when we express the vectors of the frame in a particular local basis (= local trivialization) α we get an element $g \in G$ such that $p = [(x,g)_\alpha]$. The columns of g_α are the frame vectors expressed in this local basis α, and when we change to a new local basis β these frame vector components transform appropriately. The associated principal fibre bundle of a vector bundle is also called the *frame bundle*.

If we have a principal G-bundle $P(\pi, B, G)$ we can associate to it a fibre G-bundle $\hat{E}(\hat{\pi}, B, F, G, \Phi)$, but not in a unique way – we have to choose a fibre F and a left group action Φ on it. To construct this associated fibre G-bundle, we take the total space to be:

$$\hat{E} = P \times F / \sim ,$$

where $(p_1, f_1) \sim (p_2, f_2)$ iff there exists a $g \in G$ such that $p_2 = p_1 \cdot g$ and $f_2 = \Phi(g^{-1}, f_1)$. The projection is simply $\hat{\pi}((p,f)) = \pi(p)$. Alternatively, we could have define $\hat{E}$ analogously to the previous construction of a principal G-bundle from a fibre G-bundle using its local trivializations. The transition functions would have stayed the same, as in $g_{\alpha\beta} \to \Phi_{g_{\alpha\beta}}$. One noteworthy thing about this construction is that in the process we lost the notion of a canonical right translation $\tilde{R}$ that would act on the total space $\hat{E}$. In the case of an associated vector bundle, for the construction we need a representation $\rho\colon G \to \mathrm{GL}(V)$ over some vector space V.

Finally, we would just like to note that an important result from the theory of bundle reduction of vector bundles. According to this theory, we can without any loss of generality restrict our structure group to be the unitary group $\mathrm{U}(N)$ for complex vector bundles of rank N or the orthogonal group $\mathrm{O}(N)$ for real vector bundles of rank N. In other words, we can always choose a complete set of local trivializations of a complex (real) vector bundle for which all the transition functions act like elements of $\mathrm{U}(N)$ ($\mathrm{O}(N)$).

B. Ehresmann connection

A connection is a systematic way of connecting fibres belonging to different points of the base space. In general, the way we connect two fibres will depend on the path in base space that we use to connect the two corresponding base points. The most common way of defining a connection is by introducing a covariant derivative. However, to define a covariant derivative the fibre bundle has to have a linear structure, that is, be a vector bundle. In this section we shall generalize the notion of a connection to general fibre bundles.

Let $E(\pi, B, F)$ be a fibre bundle. Consider a piecewise smooth curve $\gamma\colon [0,1] \to B$ in the base space. Then a connection, in its most general form, is a rule for transporting elements of the initial fibre $E_{\gamma(0)}$ along the path to the fibre $E_{\gamma(1)}$ at the other end. Formally, it defines a parallel transport map:

$$\mathbf{T}_\gamma\colon E_{\gamma(0)} \to E_{\gamma(1)} , \tag{27}$$

that is a fibre diffeomorphism, that continuously depends on γ, and that for piecewise smooth paths satisfies:

$$\mathbf{T}_{\gamma_2 * \gamma_1} = \mathbf{T}_{\gamma_2} \circ \mathbf{T}_{\gamma_1} ,$$
$$\mathbf{T}_{\gamma^{-1}} = \mathbf{T}_\gamma^{-1} ,$$

wher $*$ deontes the concatenation of two paths and $^{-1}$ the inversion of paths [24]. Additionally, the parallel transport map does not depend on the parameterization of γ, i.e., if $\lambda\colon [0,1] \to [0,1]$ is a smooth monotonously increasing function then $\mathbf{T}_\gamma = \mathbf{T}_{\gamma\circ\lambda}$.

If we choose a particular initial $p \in E_{\gamma(0)}$ then our parallel transport operator allows us to define a unique $\tilde{\gamma}\colon [0,1] \to E$ that starts at $\tilde{\gamma}(0) = p$, for every $t \in [0,1]$ satisfies $\pi(\tilde{\gamma}(t)) = \gamma(t)$ and finishes at $\tilde{\gamma}(1) = \mathbf{T}_\gamma(x)$. Explicitly, we have $\tilde{\gamma}(s) = \mathbf{T}_{\gamma_s}(p)$, where we have used the partial paths of the base space $\gamma_s\colon [0,1] \to B$ defined as $\gamma_s(t) = \gamma(st)$. Thus, a connection gives us a rule for *lifting* curves in the base space B to curves in the total space E. The next natural question is what structure do we need to give the fibre bundle if we want to construct a connection on it? Or, in other words, how do we uniquely determine how to lift curves? To answer this we will need two more concepts: that of a vertical and horizontal subspace.

The projection $\pi\colon E \to B$ allows us to define a pushforward $\pi_* = \mathrm{d}\pi : TE \to TB$ of vectors tangent to the total space to vectors tangent to the base space. Let $p \in E$ be a point in the total space, and T_pE the vector space tangent to p. Then the vertical subspace V_pE of T_pE is by definition the kernel of the pushforward $\mathrm{d}\pi$ at p:

$$V_pE := \ker \mathrm{d}\pi \,|_p .$$

The horizontal subspace H_pE of T_pE that is complementary to the verticle subspace V_pE in the sense that $T_pE = V_pE \oplus_p H_pE$, on the other hand, is not uniquely

defined [25]. As it turns out, this choice of horizontal subspace is sufficient for defining how to lift curves from the base to the total space!

An Ehresmann connection is a smooth assignment of horizontal subspaces $H_pE \leq T_pE$ to every point $p \in E$. They are traverse to the verticles subspaces V_pE and complementary in the sense that $T_pE = V_pE \oplus_p H_pE$. This geometric structure allows us to uniquely decompose every vector $v \in T_pE$ as:

$$v = \operatorname{hor} v + \operatorname{ver} v\,,$$

where $\operatorname{hor} v \in H_pE$ and $\operatorname{ver} v \in V_pE$ are the horizontal and vertical parts, respectively. Smoothness of assigning horizontal subspaces means that if we have a smooth vector field $X \in \mathfrak{X}(E)$ then the vector field $\operatorname{hor} X$ is also smooth. Furthermore, we can also restrict the pushforward of the projection to the horizontal subspace, making it a vector space isomorphism:

$$\begin{aligned} &\mathrm{d}\pi_H : TH \to TB\,,\\ &H_pE \ni v \mapsto \mathrm{d}\pi(v) \in T_pB\,. \end{aligned}$$

To see how this geometric structure allows us to define lifting of curves, let $\gamma\colon [0,1] \to B$ be a smooth curve in the base space. Then by demanding that the lifted curve $\tilde{\gamma}\colon [0,1] \to E$ starts at $\tilde{\gamma}(0) = p \in E_{\gamma(0)}$, and at every point of its trajectory it satisfies:

$$\begin{aligned} \operatorname{ver} \frac{\mathrm{d}\tilde{\gamma}}{\mathrm{d}t} &= 0\,,\\ \operatorname{hor} \frac{\mathrm{d}\tilde{\gamma}}{\mathrm{d}t} &= \mathrm{d}\pi_H^{-1}\left(\frac{\mathrm{d}\gamma}{\mathrm{d}t}\right)\,. \end{aligned}$$

we have specified an initial value problem that by the Picard–Lindelöf theorem has a unique solution. The lifted $\tilde{\gamma}$ of γ we shall call the *horizontal lift* of γ. The previous construction can easily be generalized to piecewise smooth paths γ. It is easy to see that the parallel transport map $\mathbf{T}$ induced by this procedure satisfies all the needed requirements mentioned after (27).

An alternative way of specifying an Ehresmann connection is via a 1-form on the tangent bundle of the total space TE with values in the verticle subbundle VE, or, alternatively, by specifying a global section of the endomorphism bundle $\operatorname{End}(TE)$, since $T^*E \otimes VE \cong \operatorname{End}(TE)$. We define the *connection 1-form* $\mathcal{A}$ as a smooth linear map:

$$\begin{aligned} &\mathcal{A}\colon TE \to VE\,,\\ &T_pE \ni v \mapsto \operatorname{ver} v \in V_pE\,. \end{aligned} \tag{28}$$

The horizontal subspace we may write as $H_pE = \ker \mathcal{A}|_p$. The horizontal lift $\tilde{\gamma}$ of γ is determined by the equation:

$$\mathcal{A}\big(\dot{\tilde{\gamma}}(t)\big) = 0\,,$$

since the condition $\pi(\tilde{\gamma}(t)) = \gamma(t)$ implies $\pi(\dot{\tilde{\gamma}}(t)) = \dot{\gamma}(t)$, so we do not need to specify the horizontal part of $\dot{\tilde{\gamma}}(t)$ explicitly.

C. Principal Ehresmann connection

For the case of a principal G-bundle $P(\pi, B, G)$ we put further restriction on the Ehresmann connection. In particular, it has to be compatible with the group structure. For the parallel transport map $\mathbf{T}$ this means that for every path γ in the base space and $g \in G$ we demand that:

$$\mathbf{T}_\gamma \circ \tilde{R}_g = \tilde{R}_g \circ \mathbf{T}_\gamma\,. \tag{29}$$

With $\gamma(0) = p$, $\gamma(1) = q$, and $P_{p\cdot g} = P_p$, we can express this condition as a commutative diagram:

$$\begin{array}{ccc} P_p & \xrightarrow{\mathbf{T}_\gamma} & P_q \\ {\scriptstyle \tilde{R}_g}\downarrow & & \downarrow{\scriptstyle \tilde{R}_g} \\ P_{p\cdot g} & \xrightarrow{\mathbf{T}_\gamma} & P_{p\cdot q} \end{array}$$

In words, if we right translate a point in the initial fibre by g and parallel transport it along a curve in base space γ we get the same result as when we first parallel transport and then right translating by g in the final fibre. This is equivalent to demanding that the assignment of horizontal subspaces for all $p \in P$ and $g \in G$ satisfy:

$$H_{p\cdot g}P = \tilde{R}_{g*}(H_pP)\,. \tag{30}$$

The connection 1-form we reformulate as a Lie algebra-valued 1-form on the tangent space of the total space. To see how, we remind the reader that the vertical subspace V_pP can be canonically associated with the tangent space T_pP_x of the corresponding fibre, where $x = \pi(p)$. Since the fibre is diffeomorphic to the structure group G, we can pullback using left translation the elements of $T_pP_x \cong T_pG$ to the identity $T_eG \cong \mathfrak{g}$, i.e., the Lie algebra. Spelling this out explicitly let $(U_\alpha, \varphi_\alpha)$ be a local trivialization and $p \in P$ a point with $\varphi_\alpha(p) = (x, g)$. Then the pushforward:

$$\varphi_{\alpha *}\colon TP|_{\pi^{-1}(U_\alpha)} \to TB|_{U_\alpha} \times TG\,,$$

when restricted to a point defines a vector space isomorphism:

$$\varphi_{\alpha *}|_p\colon T_pP \to T_xB \oplus T_gG\,.$$

When we further restrict the domain to only the vertical subspace we get an isomorphism $\varphi_{\alpha *}|_p^V : V_pP \to T_gG$. Left translation at the point g allows us to pullback to the Lie algebra, $L_g^* = L_{g^{-1}*}\colon T_gG \to T_eG$. Thus using the old connection 1-form $\mathcal{A}'$ we define a new one as:

$$\begin{aligned} &\mathcal{A}\colon TP \to \mathfrak{g}\,,\\ &T_pP \ni v \mapsto L_g^* \circ \varphi_{\alpha *}|_p^V \circ \mathcal{A}'_p(v)\,, \end{aligned} \tag{31}$$

where $\varphi_\alpha(p) = (\pi(p), g)$, and $\pi(p) \in U_\alpha$.

We can also use a manifestly local trivalization-invariant definition for $\mathcal{A}$. Let $\xi \in \mathfrak{g}$ be a Lie algebra vector. Then to ξ we can attribute the unique infinitesimal

generator of the right translation $\tilde{R}$ along ξ $\mathbf{X}_\xi \in \mathfrak{X}(P)$ that is defined as:

$$\mathbf{X}_\xi(p) := \frac{\mathrm{d}}{\mathrm{d}t}\tilde{R}(\mathrm{e}^{t\xi}, p)\Big|_{t=0}.$$

Since the canonical right action $\tilde{R}$ acts along the fibres we have $\mathbf{X}_\xi(p) \in V_pP$. In fact, for every $p \in P$ the map:

$$\begin{aligned} &Z_p \colon \mathfrak{g} \to V_pP\,, \\ &\mathfrak{g} \ni \xi \mapsto \mathbf{X}_\xi(p) \in V_pP\,, \end{aligned}$$

is a vector space isomorphism that we can use to define the connection 1-forms as:

$$\begin{aligned} &\mathcal{A} \colon TP \to \mathfrak{g}\,, \\ &T_pP \ni v \mapsto Z_p^{-1}\mathcal{A}'_p(v)\,. \end{aligned} \tag{32}$$

The proof of the equivalence of definitions (31) and (32) is given in the appendix E.

How does this connection 1-form transform when we pull it back using the right action $\tilde{R}$? The answer can be expressed using the adjoint representation as:

$$\begin{aligned} \tilde{R}_g^*\mathcal{A} = \mathrm{Ad}_{g^{-1}}\mathcal{A}\,,\ \text{or with } v \in T_pP \\ \mathcal{A}_{p\cdot g}(\tilde{R}_{g*}v) = \mathrm{Ad}_{g^{-1}}\big(\mathcal{A}(v)\big)\,. \end{aligned} \tag{33}$$

The proof of this is given in the appendix E.

The curvature 2-form measures how much the parallel transport along an infinitesimal square spanned by two vectors deviates from the identity. The curvature 2-form is defined as:

$$\begin{aligned} &\mathcal{F} \colon TP \times TP \to \mathfrak{g}\,, \\ &\mathcal{F} := \mathrm{d}\mathcal{A} + \frac{1}{2}[\mathcal{A}, \mathcal{A}]\,, \end{aligned} \tag{34}$$

where $[\,,\,]$ is the Lie bracket of $\mathfrak{g}$. In case the structure group is a matrix group, we can also write $\mathcal{A}$ as:

$$\mathcal{F} = \mathrm{d}\mathcal{A} + \mathcal{A} \wedge \mathcal{A}\,.$$

When the curve in base space γ begins and ends at the same point, i.e., $\gamma(0) = \gamma(1) = x_0$, the resulting parallel transport operator $\mathbf{T}_\gamma$ is a transformation of the initial (= final) fibre P_{x_0} in to itself. Thus, if we are given a point $p_0 \in P_{x_0}$, and the horizontal lift $\tilde{\gamma}$ of γ that starts at $\tilde{\gamma}(0) = p_0$, the final point of $\tilde{\gamma}$ can be expressed as:

$$\tilde{\gamma}(1) = \mathbf{T}_\gamma(p_0) = p_0 \cdot \Phi(\tilde{\gamma})\,.$$

This structure group element $\Phi(\tilde{\gamma}) \in G$ is the holonomy of the curve $\tilde{\gamma}$ with respect to $\mathcal{A}$. From equation (29) it follows that for a horizontal lift $\tilde{\gamma}'$ that starts at $\tilde{\gamma}'(0) = p_0 \cdot g$, the corresponding holonomy is:

$$\Phi(\tilde{\gamma}') = g^{-1} \cdot \Phi(\tilde{\gamma}) \cdot g\,.$$

Local connection 1-forms

Coming down from these abstract definitions, we would like to make practical calculations using the connection 1-form $\mathcal{A}$. This is done by introducing a local section $s \colon U \to P$, using which we define the local connection 1-form A_s as:

$$\begin{aligned} A_s \colon TB|_U \to \mathfrak{g}\,, \\ A_s := s^*(\mathcal{A})\,. \end{aligned} \tag{35}$$

This connection A_s is a $\mathfrak{g}$-valued 1-form on TB. Similarly, we define the local curvature 2-form F_s as:

$$\begin{aligned} F_s \colon TB|_U \times TB|_U \to \mathfrak{g}\,, \\ F_s := s^*(\mathcal{F})\,, \end{aligned} \tag{36}$$

that is a $\mathfrak{g}$-valued 2-form on TB. Hence, we have moved from 1-forms and 2-forms on the total space to 1-forms and 2-forms on the base space. The sacrifice we made during this transition is that the connections A_s and curvatures F_s are now defined only locally, and in general cannot be extended to the whole base space unless the bundle is trivial.

To see how the various local connection 1-forms are related, consider two local sections $s \colon U \to P$ and $z \colon O \to P$ that are on the intersection $U \cap O$ related by:

$$z(x) = s(x) \cdot g_{sz}(x)\,,$$

where $g_{sz} \colon U \cap O \to G$. In the appendix E we show that the pushforwards of these sections are related as:

$$z_*(v) = \tilde{R}_{g_{sz}(x)*}s_*(v) + Z_{z(x)}g_{sz}^{-1}(x)\,\mathrm{d}g_{sz}\,(v)\,, \tag{37}$$

for every $x \in U \cap O$ and $v \in T_xB$. If we act on this identity from the left with $\mathcal{A}$ and use equation (33), we get the desired transformation law for the local connection 1-forms:

$$A_z(v) = \mathrm{Ad}_{g_{sz}^{-1}(x)}\,A_s(v) + g_{sz}^{-1}\,\mathrm{d}g_{sz}\,(v)\,. \tag{38}$$

The second term of this transformation law is to be interpreted as meaning:

$$g_{sz}^{-1}\,\mathrm{d}g_{sz}\,(v) := \frac{\mathrm{d}}{\mathrm{d}t}\Big[g_{sz}^{-1}(x)g_{sz}\big(\gamma_v(t)\big)\Big]\Big|_{t=0}\,,$$

where $x \in B$, $v \in T_xB$, and $\gamma_v(t) \colon \langle -1, 1\rangle \to B$ is a curve that is tangential to v at time zero, i.e., $\gamma_v(0) = x$ and $\dot{\gamma}_v(0) = v$. Clearly, for $t = 0$ the quantity in the square brackets is equal to e, thus by taking the differential of this map at $t = 0$ we arrive at an element of the tangent space at e, i.e., an element of the Lie algebra $\mathfrak{g} \cong T_eG$. A more lengthy calculation (that in the case of a matrix group is straightforward) shows that the local curvature 2-forms are related according to:

$$F_z(v) = \mathrm{Ad}_{g_{sz}^{-1}(x)}\,F_s(v)\,. \tag{39}$$

For principal G-bundles, from local section one can construct local trivializations in the following way. Let $s\colon U_s \to P$ be a local section. Then the associated local trivialization (U_s, φ_s) is defined as covering the same subset of the base space, while $\varphi_s\colon \pi^{-1}(U_s) \to U_s \times G$ acts like $\varphi_s(p) = (x, g)$, where $x = \pi(p)$ and $g \in G$ is the unique element for which $s(x)\cdot g = p$. Conversely, for every local trivialization $(U_\alpha, \varphi_\alpha)$ we can define the canonical local section $\varphi_\alpha\colon U_\alpha \to P$ as $s_\alpha(x) := \varphi_\alpha^{-1}((x, e))$. From these definitions two transition relations follow:

$$\varphi_\alpha(p) = g_{\alpha\beta}(x)\cdot\varphi_\beta(p)\,,$$
$$s_\beta(x) = s_\alpha(x)\cdot g_{\alpha\beta}(x)\,,$$

that are true for all $x \in U_\alpha \cap U_\beta$ with $x = \pi(p)$. The local connection 1-form and curvature 2-form of a local trivialization $(U_\alpha, \varphi_\alpha, s_\alpha)$ we shall designate $A_{(\alpha)}$ and $F_{(\alpha)}$, where the bracket around α reminds us that they are not a components.

Using these local connection 1-forms on the base space we can define a horizontal lift. Let $\gamma\colon [0,1] \to B$ be a smooth path, and $\{(U_\alpha, \varphi_\alpha, s_\alpha)\}$ a complete set of local trivialization. We first divide the path γ in to segments γ_α completely contained in one local trivialization. For each segment we define the horizontal lift $\tilde\gamma_\alpha\colon [0,1] \to P$ as:

$$\tilde\gamma_\alpha(t) = s_\alpha(\gamma_\alpha(t))\cdot g_\alpha(t)\,,$$

where $g_\alpha\colon [0,1] \to G$ is determined by the initial condition that $\tilde\gamma_\alpha(0) = \tilde\gamma_\beta(1)$ (where β is the previous local trivialization) and the differential equation:

$$\frac{\mathrm{d}g_\alpha}{\mathrm{d}t} = -A_{(\alpha)}\big(\dot\gamma_\alpha(t)\big)\cdot g_\alpha(t)\,.$$

The explicit solution can formally be written as a path-ordered exponential:

$$g_\alpha(t) = \mathcal{P}\exp\left(-\int_{\gamma_\alpha} A_{(\alpha)}\right)\cdot g_\alpha(0)\,.$$

To get the final horizontal lift we simply concatenate the individual segments.

Relation to the linear connection

We end our discussion of Ehresmann connections by relating them to the familiar connections on vector bundles, also called linear connections.

Let $\hat E(\hat\pi, B, k^N, G)$ be an associated vector bundle of the principal bundle $P(\pi, B, G)$ induce by the representation $\rho\colon G \to \mathrm{GL}(N,k)$, where $k = \mathbb{R}$ or $\mathbb{C}$. Hats will be used to designate quantities related to the associated vector bundles. A complete set of local trivializations of the principal bundle $\{(U_\alpha, \varphi_\alpha, s_\alpha)\}$ is then associated to a complete set of local trivializations of the vector bundle $\{(U_\alpha, \hat\varphi_\alpha)\}$, with the transition functions related according to $\hat\varphi_\alpha \circ \hat\varphi_\beta^{-1}|_x = \rho(g_{\alpha\beta}(x)) \equiv \hat g_{\alpha\beta}(x)$.

Furthermore, in the associated vector bundle to every local trivialization we can associate a canonical basis of the corresponding fibres by choosing N local section $\hat s_{\alpha,i}(x) = \hat\varphi_\alpha^{-1}((x, e_i))$, where $e_i \in k^N$ is simply the vector with the i-th component equal to one and all others zero. This is analogous to the canonical local section s_α that we defined for the principal fibre bundle. A change of trivialization lead to a change of basis:

$$\varphi_\alpha(s_{\beta,i}(x)) = \hat g_{\alpha\beta}(x)\cdot\varphi_\beta(s_{\beta,i}(x))\,.$$

Since the associated vector bundle doesn't have a local trivialization-independent way of multiplying sections by structure group elements (i.e., their representing matrices), the best we can do is write:

$$s_{\beta,i}(x) = s_{\alpha,j}(x)\hat g_{\alpha\beta,ji}(x)\,,$$

where $\hat g_{\alpha\beta,ji}$ are the matrix elements of $\hat g_{\alpha\beta}$, and the sum of the index j is implied.

To a representation (ρ, V) there is also associated a pushforward (differential) $\rho_* = \mathrm{d}\rho : \mathfrak{g} \to \mathfrak{gl}(V,k)$. Using this representation of the Lie algebra $\mathfrak{g}$, the local connection 1-form $A_{(\alpha)}$ of some local trivialization α on the principal bundle can be pushed forward to a local connection 1-form $\hat A_{(\alpha)} = \rho_*\big(A_{(\alpha)}\big)$ on the vector bundle, and analogously for the curvature 2-forms $\hat F_{(\alpha)} = \rho_*\big(F_{(\alpha)}\big)$. This allows us to define a covariant derivative. A covariant derivative is by definition a map:

$$D\colon\ \mathfrak{X}(B)\times\Gamma(E) \to \Gamma(E)\,,$$
$$\mathfrak{X}(B)\times\Gamma(E) \ni (v,s) \mapsto D(v,s) = D_v(s)\,,$$

that is $C^\infty(B)$-linear in the vector field v, $\mathbb{R}$-linear in the section s, and satisfies the Leibniz rule:

$$D_v(fs) = v(f)s + fD_v(s)\,,$$

for all $v \in \mathfrak{X}(B)$, $s \in \Gamma(E)$, and smooth functions $f \in C^\infty(B)$. The covariant derivative associated to the local connection 1-form $\hat A_\alpha$ we define as acting on a local section $\psi = \psi^i \hat s_{\alpha,i} \in \Gamma(U_\alpha, E)$ as:

$$D_v\psi = v(\psi^i)\hat s_{\alpha,i} + \psi^i\varphi_\alpha^{-1}\left(\hat A_{(\alpha)}(v)\cdot e_i\right)\,,$$

where the summation of the index i over $1, 2, \ldots, N$ is implied.

To simplify the previous expressions, we drop the α label for the particular local trivialization, and presume that the choice of the local section $s_i = s_{\alpha,i}$ is known. The dual section we shall denote $s_*^i(s_j) = \delta^i_j$. We also presume that some coordinates x^μ of the base space B are given, using which we can express vector fields as $v(x) = v^\mu(x)\partial_\mu$ with $\partial_\mu = \partial/\partial x^\mu$. The summation of the indices $\mu, \nu = 1, 2, \ldots, \dim B$ and $i, j, k = 1, 2, \ldots, N$ will follow Einstein's convection. For the matrix elements of $A(v) = v^\mu A_\mu = A_{(\alpha)}(v)$ we write $A^i{}_j(v) = v^\mu A^i_{\mu j}$. If we just write A, then that matrix is suppose to be understood as

acting on column-vectors $\vec{\psi}$ with components ψ^i of some local section $\psi = \psi^i s_i$. With all of this in place, we have:

$$\begin{aligned} D_v\psi &= (D_v\psi)^i\, s_i = v^\mu\, (D_\mu\psi)^i\, s_i\,, \\ (D_v\psi)^i &= D_v\psi^i = v(\psi^i) + A^i{}_j(v)\psi^j\,, \\ (D_\mu\psi)^i &= D_\mu\psi^i = \partial_\mu(\psi^i) + A^i_{\mu j}\psi^j\,. \end{aligned} \tag{40}$$

Moreover, we can write:

$$\begin{gathered} D = D_\mu\, \mathrm{d}x^\mu\ , \text{ with} \\ D_\mu = \partial_\mu + A_\mu\,, \quad A_\mu = A^i_{\mu j} s_i \otimes s^j_*\,. \end{gathered}$$

Upon a change of local sections $s_i \to s_{i'}$:

$$s_{i'} = s_j g_{ji'}\,, \quad \psi^{i'} = g^{-1}_{i'j}\psi^j\,,$$

a straightforward calculation shows that the transformation for the covariant derivative, connection 1-form, and curvature 2-form are:

$$\begin{aligned} D'_\mu &= \partial_\mu + A'_\mu = g^{-1} D_\mu g\,, \\ A'_\mu &= g^{-1} A_\mu g + g^{-1}\partial_\mu(g)\,, \\ F'_{\mu\nu} &= [D'_\mu, D'_\nu] = g^{-1} F_{\mu\nu} g\,. \end{aligned} \tag{41}$$

Primes mark the quantities of this new basis, and all of the above expression are to be interpreted as acting on column-vectors $\vec{\psi}'$ made of the components $\psi^{i'}$ in this new basis.

The equation that determines the horizontal lift $\psi\colon [0,1] \to \hat{E}$ of some curve $\gamma(t) = \hat{\pi}(\psi(t))$ in the base space is:

$$D_{\dot\gamma(t)}\psi^i = \frac{\mathrm{d}\psi^i}{\mathrm{d}t} + A^i{}_j(\dot\gamma(t))\psi^j = 0\,.$$

As long as we stay within one local trivialization (i.e., within the domain of the local sections s_i), we can write the formal solution for the parallel transport equation as:

$$\vec{\psi}(t) = \mathcal{P}\exp\left(-\int_0^t \mathrm{d}t'\, A(\dot\gamma(t'))\right)\vec{\psi}(0)\,.$$

VIII. APPLICATION OF THE MATHEMATICAL FORMALISM

We have seen geometrical phases appearing in physics in two ways. In the first case, we had a physical system whose parameters we varied adiabatically, and as we varied them the system stayed in the corresponding eigenspace of the Hamiltonian. This naturally lends itself to be interpreted as having a vector bundle over the parameter space. The fibres are the respective eigenspaces, adiabatic evolution becomes parallel transport, and the adiabatic phase is a holonomy. This interpretation we shall call Berry-Simon's interpretation.

In the second case, we had an arbitrary system that evolved cyclically, and to the closed path in the projective Hilbert space we attributed a geometric phase. The adiabatic phase turned out to be a special case of this geometric phase. According to the Aharonov-Anandan's interpretation, we introduce a vector bundle over the projective Hilbert space. The fibres are normalized states that share the same projector, a natural connection is introduced, and the Aharonov-Anandan's phase becomes a holonomy of this connection.

A. Berry-Simon's approach

As one can see from our derivation of Berry's phase, the only limitation on the parameter space that we needed was that it locally resembles $\mathbb{R}^N$. Naturally, we generalize our previous discussion of Berry's phase by taking the parameter space to be a connected smooth N-manifold B. The parameters R^μ are now to be interpreted as local coordinates on this manifold.

The space of physical states is of course a separable complex Hilbert space $\mathcal{H}$, and the Hamiltonian is an essentially self-adjoint operator $\hat{H}$ whose domain is a dense linear subspace of $\mathcal{H}$. In our case we shall be interested in a Hamiltonian that is a smooth operator-valued function on the parameter space B. The Hamiltonian will in general have a discreet spectrum whose eigenvectors live in $\mathcal{H}$ and a continuous spectrum whose eigenvectors live in the dual $\mathcal{H}^*$. (For those unfamiliar with this mathematically rigorous expression of quantum mechanics, we recommend [15] for an accessible introduction.) We limit ourselves to one specific eigenspace of the Hamiltonian $\mathcal{H}_n \leq \mathcal{H}$ that is an element of the discreet spectrum and whose energy E_n is a finite distance away from the rest of the spectrum (i.e., there's a gap) throughout the parameter space. This implies that the dimension of the eigenspace $N = \dim \mathcal{H}_n$ is constant throughout the parameter space. For convenience we shall redefine the Hamiltonian $\hat{H}(R^\mu) \to \hat{H}(R^\mu) - E_n(R^\mu)$ so that the n-th energy is now zero, and the eigenspace $\mathcal{H}_n$ is equal to the kernel $\ker \hat{H}$.

Now we are in a position to define the vector bundle of eigenspaces over the parameter space with a structure group $\mathrm{U}(N)$. As the base manifold we take parameter space B. The fibre over each point $p \in B$ is the eigenspace $\mathcal{H}_n(p)$. The total space E we define as:

$$E := \bigsqcup_{p\in B} \{p\} \times \mathcal{H}_n(p)\,,$$

and the projection $\pi\colon E \to B$ by $\pi(p, |\psi\rangle) = p$. The fibres over a point $p \in B$ we shall abbreviate as $E_p = \pi^{-1}(p)$. To define a local trivialization around some arbitrary $p \in B$, we choose an open neighborhood U_p of that point and a orthonormalized basis $\{|\varphi_i\rangle : U_p \to \mathcal{H}\}$ that smoothly attributes to every $q \in U_p$ normalized vectors $|\varphi_i(q)\rangle \in \mathcal{H}_n(q)$, $i = 1, 2, \ldots, N$, in the corresponding eignespace. Using this basis, we can locally express every vector in

$\mathcal{H}_n$ as a complex vector $\mathbb{C}^N$, allowing us to define:

$$f_p \colon \pi^{-1}(U_p) \to U_p \times \mathbb{C}^N \,, \\ (q, |\psi\rangle) \mapsto (q, v(q)) \,,$$

where the components of the vector $v(q)$ are $v_i(q) = \langle\varphi_i(q)|\psi\rangle$.

On the intersection $U \cap U'$ between two local trivializations (f, U) and (f', U') we can ask ourselves how does the function $f' \circ f^{-1}$ act? We see that for every $p \in U \cap U'$ and $|\psi\rangle \in \mathcal{H}_n(p)$ it acts as:

$$\langle\varphi_i(p)|\psi\rangle \mapsto \langle\varphi'_i(p)|\psi\rangle = \sum_{j=1}^{N} \langle\varphi'_i(p)|\varphi_j(p)\rangle \langle\varphi_j(p)|\psi\rangle \ .$$

Since the local bases were demanded to be orthonormalized, if follows that the matrix with components $\langle\varphi'_i(r)|\varphi_j(p)\rangle$ is in $\mathrm{U}(N)$, i.e., the transition functions act like elements of the structure group $\mathrm{U}(N)$ in the canonical representation. It is easily seen that these transition functions satisfy the identity, inverse and cocycle conditions. Thus, we have defined a vector $\mathrm{U}(N)$-bundle $E(\pi, B, \mathbb{C}^N, \mathrm{U}(N))$, to which we attribute an associated principal $\mathrm{U}(N)$-bundle $P(\pi, B, \mathrm{U}(N))$. Alternatively, we could have defined this vector bundle as a subbundle of the trivial bundle $B \times \mathcal{H}$.

The fact that the state space $\mathcal{H}$ has a scalar product defined on it allows us to define a canonical or natural connection on the vector bundle $E \to B$ or, equivalently, on the principal bundle $P \to B$.

To see how we can do this, let us start with the simplest case of $N = 1$, in which case the eigenspaces $\mathcal{H}_n$ are non-degenerate. Recall that the principal bundle can be interpreted as a frame bundle of the vector space. In our case this means that every point $p \in P$ above $x = \pi(p)$ we can interpret as a normalized vector in $\mathcal{H}_n(x)$. To define an Ehresmann connection of the principal bundle, we have to attribute to every vector $v_p \in T_pP$ an element of the Lie algebra $\mathfrak{u}(1) \cong \mathrm{i}\mathbb{R}$. Since the scalar product $\langle\,|\,\rangle : \mathcal{H} \times \mathcal{H} \to \mathbb{C}$ allows us to attribute to two vectors that live in different fibres a scalar, we simply define the connection 1-form $\mathcal{A} \colon TP \to \mathfrak{u}(1)$ as:

$$\mathcal{A}(v_p) := \frac{\mathrm{d}}{\mathrm{d}t} \langle p|\gamma_v(t)\rangle \Big|_{t=0} \,,$$

where γ_v is a path in P tangential to $v_p \in T_pP$ at $t = 0$. Since both p and $\gamma_v(t)$ are normalized vectors, their scalar product is an element of $\mathrm{U}(1)$, and the derivative of the scalar product is in $\mathfrak{u}(1)$.

The generalization of the previous construction to $N > 1$ is straightforward. Every point $p \in P$ above $x = \pi(p)$ is now an orthonormal N-tuple of vectors (ordered basis) in $\mathcal{H}_n(x)$ that we shall denote p_i, with $i = 1, 2, \ldots, N$. The $\mathfrak{u}(N)$-valued connection 1-form we define as having components:

$$\mathcal{A}^i{}_j(v) := \frac{\mathrm{d}}{\mathrm{d}t} \langle p_i|\gamma_{v,j}(t)\rangle \Big|_{t=0} \,,$$

where γ_v is a path in P tangential to $v \in T_pP$ at $t = 0$.

With connection 1-forms in place, we can define local connection 1-forms. Let $s \colon U \to P$ be a local section of the principal bundle, i.e., an orthonormalized basis of $\mathcal{H}_n$. The individual vectors we'll designate s_i. Then the local connection 1-form $A \colon TB|_U \to \mathfrak{u}(N)$ is defined as having components:

$$A^i{}_j(v_x) := \frac{\mathrm{d}}{\mathrm{d}t} \langle s_i(x)|s_j(\gamma_v(t))\rangle \Big|_{t=0} \,,$$

where $x \in U$ and γ_v is a path in B tangential to $v_x \in T_xB$ at $t = 0$. We can also define it in some coordinates x^μ of B as:

$$A^i_{\mu j}(v_x) = \langle s_i|\partial_\mu s_j\rangle \ .$$

Coming back to the initial vector bundle, the local connection 1-form is defined in the same way as for the associated principal bundle, since the representation of group element is trivial. The covariant derivative of a local section of the vector bundles $\psi = \psi^i s_i \colon U \to E$ is:

$$(D_\mu\psi)^i = \partial_\mu(\psi^i) + A^i_{\mu j}\psi^j \,.$$

Using the fact that $\psi^i = \langle s_i|\psi\rangle$, we can rewrite the covariant derivative as:

$$(D_\mu\psi)^i = \langle s_i|\partial_\mu\psi\rangle \ ,$$

which means that $D = \hat{P}_n \mathrm{d}$, with $\hat{P}_n = \sum_i |s_i\rangle\langle s_i|$ being the projector to the eigenspace $\mathcal{H}_n$. Explicitly, we have:

$$D_v\psi = \hat{P}_n \, \mathrm{d}\psi \, (v) = \sum_{i=1}^{N} |s_i\rangle \langle s_i|v(\psi)\rangle \ .$$

It is easy to see that the local connection 1-form A defined here is the same as Berry's (6) and Wilczek-Zee's (14), up to a conventional imaginary constant and transposition. The parallel transport defined by the covariant derivative D coincides with adiabatic evolution up to a dynamical phase that we removed with a redefinition of the Hamiltonian. The holonomies of closed curves in the base space are equal to Berry's (8) and Wilczek-Zee's (15) phase.

B. Aharonov-Anandan's approach

In the Aharonov-Anandan's approach, as the base space we take the space of physical state, i.e., the quantum phase space that has the mathematical structure of a projective Hilbert space. We previously noted that, in general, this space is infinite-dimensional, and, as such, mathematically more demanding. In the section on Aharonov-Anandan's phase we introduce it as the quotient space:

$$\mathcal{P}(\mathcal{H}) = \mathcal{S}(\mathcal{H}) / \sim \,,$$

where two vectors are equivalent if they differ by a phase. Since the original sphere $\mathcal{S}(\mathcal{H})$ has a well-defined topology, this quotient space inherits a topology as well. Moreover, one can also give $\mathcal{P}(\mathcal{H})$ the structure of an infinite-dimensional manifold.

There is also an alternative way of introducing the quantum phase space that rests on first taking the case of a finit number of possible states whose superposition we take, and then taking the limit to infinity. In particular, if we have $\mathcal{H} = \mathbb{C}^{N+1}$ then the projective Hilbert space is equal to the complex projective space $\mathcal{P}(\mathcal{H}) \cong \mathbb{C}P^N$. For projective complex spaces the following inclusion is true:

$$\mathbb{C}P^1 \subset \mathbb{C}P^2 \subset \cdots \subset \mathbb{C}P^{N-1} \subset \mathbb{C}P^N \subset \cdots ,$$

that allows us to write:

$$\mathbb{C}P^N = \bigcup_{n=1}^{N} \mathbb{C}P^n .$$

By taking the *inductive* or *direct* limit, we may generalize and define:

$$\mathbb{C}P^\infty := \bigcup_{n=1}^{\infty} \mathbb{C}P^n .$$

This only defines $\mathbb{C}P^\infty$ as a set of points, without any topology or manifold structure. We furthermore give $\mathbb{C}P^\infty$ a topology by defining the open subsets to be the unions of open subsets of $\mathbb{C}P^n \subset \mathbb{C}P^\infty$, for all $n = 1, 2, \ldots$.

These two ways of defining the quantum phase space are inequivalent. Fortunately, in the next step when we define a principal U(1)-bundle over these two variant, they will be in a one-to-one correspondence.

Skimming over the mathematical details, we define the Aharonov-Anandan's principal U(1)-bundle as having a base space $\mathcal{P}(\mathcal{H})$ and total space $\mathcal{S}(\mathcal{H})$. Points in $\mathcal{P}(\mathcal{H})$ we shall describe with projectors, while points in $\mathcal{S}(\mathcal{H})$ we shall describe with normalized state vectors. The projection π we define as $\pi(|\psi\rangle) = \hat{P}_\psi = |\psi\rangle\langle\psi|$. Local trivializations amount to choosing a local section. The scalar product allows us to define a natural connection 1-form $\mathcal{A}\colon T\mathcal{S}(\mathcal{H}) \to \mathfrak{u}(1)$ as:

$$\mathcal{A}(v_\varphi) := \frac{\mathrm{d}}{\mathrm{d}t} \langle\varphi|\psi(t)\rangle \Big|_{t=0} ,$$

where ψ is a path in $\mathcal{S}(\mathcal{H})$ tangential to $v_\varphi \in T_\varphi\mathcal{S}(\mathcal{H})$ at $t = 0$. The covariant derivative is $D = \hat{P}_\psi \mathrm{d}$. The holonomy of a closed curve $\mathcal{C}$ in $\mathcal{P}(\mathcal{H})$ is:

$$\Phi(\mathcal{C}) = \exp\left(- \oint_{\mathcal{C}} \langle\psi|\mathrm{d}\psi\rangle \right) ,$$

where $|\psi\rangle$ si a local section $\hat{P}_\psi \to |\psi\rangle$. This mathematically natural connection 1-form and holonomy coincides with Aharonov-Anandan's. We also see how the condition that the function over which we integrate $|\tilde{\psi}\rangle$ be periodic naturally arises from the fact that local sections have to be one-valued on $\mathcal{P}(\mathcal{H})$.

This finishes the exposition of the mathematical formalism of geometric phases. Holonomies are the desired geometrical phases, and the mathematically natural connections that we define using the scalar product equals the physical connection of interest.

IX. CONCLUSION

Having introduced the foundational physical results regarding geometrical phases, and the mathematical formalism used to describe it more abstractly, we remark that many fascinating topics have not been discussed or covered in this article, but with this background should be accessible to the readers.

Beyond the short introduction to the gauge theory of molecular physics that we gave, in [20] the reader may find a more detailed exposition of this topic, together with a fascinating discussion that relates Aharonov-Anandan's U(1)-bundle to the categorization of all principal U(1)-bundles, as well as a thorough discussion of geometric phases as they appear in condensed matter physics, the quantum Hall effect, and many-body systems. In the review article [17] a pedagogical introduction to Berry's phase as it appears in solid-state physics is given. Closer to pure theory, in [21] geometrical phases in both quantum and classical mechanics are discussed from a unified, geometric point of view at a mathematically sophisticated level. Together with review articles [12, 13], this covers the geometric formulation of quantum mechanics.

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[22] In this approximation the effective potential $\epsilon_n(\mathbf{R})$ is also modified into $\tilde{\epsilon}_n(\mathbf{R}) = \epsilon_n(\mathbf{R}) + \Phi_n(\mathbf{R})$, where the scalar gauge potential $\Phi_n(\mathbf{R})$ is defined as:

$$\Phi_n(\mathbf{R}) = \frac{\hbar^2}{2\mu} \sum_{m=\mathcal{N}+1}^{\infty} \mathbf{A}^{nm}(\mathbf{R}) \cdot \mathbf{A}^{mn}(\mathbf{R}) \,.$$

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[23] An intuitive introduction to these mathematical topics can be found in Appendix of Chapter 3 of [19], a more formal one in Chapter 5 and the Appendix of [20], a terse mathematical one in Chapter 1 of [21].

[24] The concatenation of two paths $\gamma_1, \gamma_2 \colon [0,1] \to B$ that satisfy $\gamma_1(1) = \gamma_2(0)$ is defined piecewise as $(\gamma_2 * \gamma_1)(t \leq \frac{1}{2}) := \gamma_1(2t)$ and $(\gamma_2 * \gamma_1)(t \geq \frac{1}{2}) := \gamma_2(2t-1)$. The inversion of a path $\gamma \colon [0,1] \to B$ is defined as the path $\gamma^{-1}(t) := \gamma(1-t)$.

[25] The naming of the vertical and horizontal subspace follows the usual convention of depicting fibre bundles as having a "horizontal" base space with fibres spanning along the "vertical" direction.

Appendix A: Jacobi's coordinates

The main idea of Jacobi's coordinates is to recursively combine kinetic energy terms until all the terms have been combined into relative ones and a centre of mass (CM) term that we can subsequently remove. For example, to combine kinetic term a and b we simply substitute:

$$\frac{p_a^2}{2m_a} + \frac{p_b^2}{2m_b} \longrightarrow \frac{p_{ab}^2}{2\mu_{ab}} + \frac{P_{ab}^2}{2M_{ab}} \,,$$

where $p_{ab} = -\mathrm{i}\hbar\, \partial/\partial x_{ab}$, $P_{ab} = -\mathrm{i}\hbar\, \partial/\partial X_{ab}$ and:

$$\begin{aligned} x_{ab} &= x_b - x_a \,, \quad & \mu_{ab}^{-1} &= m_a^{-1} + m_b^{-1} \,, \\ X_{ab} &= x_a + x_b \,, \quad & M_{ab} &= m_a + m_b \,. \end{aligned}$$

Next we combine the P_{ab} term with some other, e.g., P_{cd} term while retaining the relative motion terms p_{ab} and p_{cd}. We continue to do this until only relative motion terms and one centre of mass term are left. After this the individual coordinates are rescaled so that all the non-CM kinetic terms all share the same denominator μ.

There is arbitrariness in the way you can group together the various kinetic terms. In the case of three terms (a, b, c), one could first group $a-b$ and then $ab-c$, or first group $a-c$ and then $ac-b$, etc. Regardless of the order, in the end a CM term always appears. For our theoretical analysis the grouping of the terms is immaterial.

Appendix B: Lie groups and algebras

A Lie group G is a group that is also a differentiable manifold, and the group operations of multiplication and inversion are compatible with this differentiable structure. In other words, the set of group elements G is a real smooth manifold, and both multiplication $*\colon G \times G \to G$, $(g,h) \mapsto g * h$ and inversion $^{-1}\colon G \to G$, $g \mapsto g^{-1}$ are

smooth maps. Further on, multiplication will be designate by juxtaposition.

Every element $g \in G$ give rise to two diffeomorphisms, left translation by g that is defined as $L_g \colon G \to G$, $L_g(h) := gh$ and right translation by g defined as $R_g \colon G \to G$, $R_g(h) := hg$.

A smooth vector field $X \in \mathfrak{X}(G)$ is called left-invariant if it is invariant under the pushforward of all left translations, i.e., $L_{g*}X = X$ for all $g \in G$. The set of left-invariant vector fields we shall denote $\mathfrak{X}_L(G)$. Right-invariant vector fields $\mathfrak{X}_R(G)$ are analogously defined.

Let $e \in G$ be the identity. Then every smooth left-invariant vector field is uniquely determined by its value at the identity, i.e., the map $\mathfrak{X}_L(G) \ni X \mapsto X(e) \in T_eG$ is a vector space isomorphism. This is so because we can left translate the value at the identity to any point on G. Furthermore, left-invariant vector fields are closed under the commutator, therefore giving $\mathfrak{X}_L(G)$ a Lie algebra structure. This structure when pushed froward to T_eG by the aforementioned isomorphism gives T_eG a Lie bracket and makes T_eG a Lie algebra as well. Explicitly, if $X(e) = \xi$ and $Y(e) = \eta$ then $[\xi, \eta] := [X, Y](e)$. The Lie algebra of T_eG we shall mark as $\mathfrak{g}$.

To each $\xi \in \mathfrak{g}$ we can associate a one-parameter subgroup of G by the following procedure. Let $X_\xi \in \mathfrak{X}_L(G)$ be the unique left-invariant vector field that satisfies $X_\xi(e) = \xi$. Then there is a unique integral curve $g_\xi \colon \mathbb{R} \to G$ of X for which:

$$\frac{\mathrm{d}}{\mathrm{d}t} g_\xi(t) = X_\xi(g_\xi(t)) \,,$$

with the initial conditions $g_\xi(0) = e$ and $\dot{g}_\xi(0) = \xi$. Using this construction, we define the exponential map $\exp \colon \mathfrak{g} \to G$ by $\exp(\xi) = g_\xi(1)$. Conversly, we can write the one-parameter subgroup of G associated to ξ as $g_\xi(t) = \exp(t\xi)$. The previous construction of exp does not depend on whether a left- or right-invariant vector field associated to ξ was used.

To every $g \in G$ we can defined the conjugation by g function, defined as $I_g \colon G \to G$, $h \mapsto ghg^{-1}$. By taking the differential (or pushforward) of I_g at the identity we get the adjoint representation of g, $\mathrm{Ad}_g = (\mathrm{d}I_g)_e \colon \mathfrak{g} \to \mathfrak{g}$. Since Ad_g is a pushforward, it is a linear operator on $\mathfrak{g}$. Hence, the map $\mathrm{Ad} \colon G \to \mathrm{GL}(\mathfrak{g}, \mathbb{R})$, $g \mapsto \mathrm{Ad}_g$ defines a representation of the group G over the vector space $\mathfrak{g}$. In the case of a matrix group, $\mathrm{Ad}_A(B) = ABA^{-1}$ where $A \in \mathrm{GL}(N, \mathbb{R})$ and $B \in \mathfrak{gl}(N, \mathbb{R})$. By taking the the differential of the adjoint representation map Ad at the identity, we arrive at a representation of the Lie algebra: $\mathrm{ad} = (\mathrm{d}\,\mathrm{Ad})_e \colon \mathfrak{g} \to \mathfrak{gl}(\mathfrak{g}, \mathbb{R})$. One can show that $\mathrm{ad}_\xi(\eta) = [\xi, \eta]$. Two important identities relating the adjoint representations to the exponential map are:

$$\begin{aligned} I_g(\exp(\xi)) &= \exp(\mathrm{Ad}_g(\xi)) \,, \\ \mathrm{Ad}_{\exp(\xi)} &= \exp(\mathrm{ad}_\xi) \,. \end{aligned}$$

Appendix C: Lie group action

Let M be a real manifold with points $x, y, \ldots \in M$ and G a real Lie group with identity e and elements $g, h, \ldots \in G$. A left action of G on M is a smooth map $\Phi \colon G \times M \to M$ that satisfies $\Phi_e(x) = x$ for all x, and $\Phi_g \circ \Phi_h = \Phi_{gh}$ for all g and h. Here we used the abbreviation $\Phi_g(x) = \Phi(g, x)$. A right action is defined in the same with the second condition replaced by $\Phi_g \circ \Phi_h = \Phi_{hg}$.

The most general group G that we can take is the group of diffeomorphism of M $\mathrm{Diff}(M)$. This infinite dimensional Lie group defines a left group action in the obvious way, $\Phi(\varphi, x) = \varphi(x)$ where $\varphi \in \mathrm{Diff}(M)$. The left (right) group action we can understood as a (anti-)homomorphism from G to $\mathrm{Diff}(G)$ by way of $G \ni g \mapsto \Phi_g \in \mathrm{Diff}(M)$.

The orbit $\mathrm{Orb}(x)$ of x we define as the set:

$$\mathrm{Orb}(x) := \{\, \Phi_g(x) \mid g \in G \,\} \subseteq M \,.$$

From the definition of a group, if follows that "being in the same orbit" defines an equivalence relation of points in M, alternatively expressed as $x \sim y$ iff there exists a g such that $y = \Phi_g(x)$. Thus orbits partition M. The set of all orbits is written as M/G and called the quotient of the action.

A point x is a fixed point of g iff $\Phi_g(x) = x$, and a subspace $A \subseteq M$ is a fixed subspace of g iff $\Phi_g(x) = x$ for all $x \in A$. A subspace $A \subseteq M$ is called invariant iff $x \in A \implies \Phi_g(x) \in A$ for all g.

The stabilizer or isotropy subgroup of Φ at x is the set:

$$\mathrm{St}(x) := \{\, g \in G \mid \Phi_g(x) = x \,\} \subseteq G \,.$$

In words, it is the set of all group elements for which x is a fixed point. A little reflection shows that $\mathrm{Orb}(x) \cong G/\,\mathrm{St}(x)$.

A group action Φ is said to be:

- transitive if there is only one orbit, i.e., for all x and y there is a g that connects them $y = \Phi_g(x)$.
- faithful (or effective) if the homomorphism $G \to \mathrm{Diff}(M)$ is injective, i.e., $g \neq h$ implies $\Phi_g \neq \Phi_h$. Equivalently, Φ is faithful iff $\Phi_g = \mathrm{id}_M$ implies $g = e$.
- free if it has no fixed points, i.e., if there exists a x such that $\Phi_g(x) = x$, then $g = e$. Equivalently, Φ is free iff $\mathrm{St}(x) = \{e\}$ for all x.

Every free action is faithful. An example of a transitive and free group action are translations over Euclidian space. An example of an transitive and faithful group action are rotations over the 2-sphere.

Using a group action Φ we can attribute to every $\xi \in \mathfrak{g}$ a vector field $\mathbf{X}_\xi \in \mathfrak{X}(M)$ called the infinitesimal generator of the action Φ along ξ. We define it as:

$$\mathbf{X}_\xi(x) := \frac{\mathrm{d}}{\mathrm{d}t} \Phi(\exp(t\xi), x)\Big|_{t=0} \,.$$

This map $\xi \mapsto \mathbf{X}_\xi$ defined for a right (left) group action Φ is a Lie algebra (anti-)homomorphism, i.e., $[\mathbf{X}_\xi, \mathbf{X}_\eta] = \pm^R_L \mathbf{X}_{[\xi,\eta]}$.

Appendix D: Fibre bundles

Fibre bundles formalize the notion of having over each point in the base space a fibre space, and generalizes the idea of a product space to space that only locally looks like a product. Every smooth fiber bundle is made of:

- three smooth manifolds: the total space E, the base space B and the standard or typical fiber F, and
- a smooth surjection (called the projection) $\pi\colon E \to B$ such that the fiber $E_x = \pi^{-1}(x)$ of every $x \in B$ is diffeomorphic to F.

The fibers E_x we typically imagine as being situated "above" the point x in the base space. The rank of the fiber bundle is defined as the dimension of the fiber as a manifold. We further demand that:

- the fiber bundle is locally trivial, i.e., locally diffeomorphic to a Cartesian product of an open subset of the base manifold with the standard fiber. In particular, there exists an open cover $\{U_\alpha\}$ of B together with diffeomorphisms (called local trivializations) $\varphi_\alpha\colon \pi^{-1}(U_\alpha) \to U_\alpha \times F$ of the form $\varphi_\alpha(p) = (\pi(p), \phi_\alpha(p))$, where $\phi_\alpha\colon \pi^{-1}(U_\alpha) \to F$ is smooth. Thus, $\pi^{-1}(U_\alpha) \cong U_\alpha \times F$. The following diagram is commutative:

$$\begin{array}{ccc} \pi^{-1}(U_\alpha) & \xrightarrow{\varphi_\alpha} & U_\alpha \times F \\ {\scriptstyle\pi}\downarrow & \swarrow_{\pi_1} & \\ U_\alpha & & \end{array}$$

- on the intersection of the local trivializations $(U_\alpha, \varphi_\alpha)$ and (U_β, φ_β) the induced transition functions $\chi_{\alpha\beta}(x) := \phi_\alpha \circ \phi_\beta^{-1}|_x\colon F \to F$ are diffeomorphisms.

Clearly, the transition functions satisfy:

- the identity condition $\chi_{\alpha\alpha}(x) = \mathrm{id}_F$ for all $x \in U_\alpha$,
- the inversion condition $\chi^{-1}_{\alpha\beta}(x) = \chi_{\beta\alpha}(x)$ for all $x \in U_\alpha \cap U_\beta$, and
- the cocycle condition $\chi_{\alpha\beta}(x) \circ \chi_{\beta\gamma}(x) \circ \chi_{\gamma\alpha}(x) = \mathrm{id}_F$ for all $x \in U_\alpha \cap U_\beta \cap U_\gamma$.

It is these transition functions that specify the global topology of the fiber bundle, and allows us to sew together the local trivializations in a consistent way. Fiber bundles, as defined above, we shall demarcate as $E(B, \pi, F)$, $F \hookrightarrow E \xrightarrow{\pi} B$ or simply $E \to B$.

A bundle morphism among two fiber bundles $E(B, \pi, F)$ and $E'(B', \pi', F')$ is a pair of smooth functions $(\Psi\colon E \to E', \psi\colon B \to B')$ that satisfies $\Psi \circ \pi' = \pi \circ \psi$. This means that Ψ maps fibres E_x to fibres $E'_{\psi(x)}$ for all $x \in B$. A morphism is an isomorphism if the smooth functions (Ψ, ψ) are also diffeomorphisms. Isomorphic bundles we shall call equivalent; this defines an equivalence relation in the category of all fibre bundles. If a property is shared among equivalent bundles, then we say that it is a topological property. An important class of isomorphisms is that of automorphisms (isomorphisms from the bundle to iteslf) that leave the base space fixed; they form a group under composition called the gauge group.

If we are given a smooth map $f\colon M \to B$, where M is a smooth manifold and B the base space of the fibre bundle $E(B, \pi, F)$, we can construct a pullbacked fibre bundle (f^*E, M, π_1, F). The pullbacked total space f^*E is defined as:

$$f^*E := \{\, (x, u) \in M \times E \mid f(x) = \pi(u) \,\},$$

while the projection $\pi_1\colon f^*E \to M$ is defined by $\pi_1((x, p)) = x$. As one can easily see, the fibres $f^*E_x = \pi_1^{-1}(x)$ are just copies of the fibres $E_{f(x)} = \pi^{-1}(f(x))$. We may also introduce the projection $\pi_2\colon f^*E \to E$ defined by $\pi_2((x, p)) = p$ that satisfies $\pi_2 \circ \pi = \pi_1 \circ f$, i.e., the following diagram commutes:

$$\begin{array}{ccc} f^*E & \xrightarrow{\pi_2} & E \\ {\scriptstyle\pi_1}\downarrow & & \downarrow{\scriptstyle\pi} \\ M & \xrightarrow{f} & B \end{array}$$

Finally, let $\{(U_\alpha, \varphi_\alpha)\}$ be a complete set of local trivializations of $E \to B$. Then the set $\{O_\alpha = f^{-1}(U_\alpha)\}$ defines an open cover of M, and we may define the corresponding local trivialization of $f^*E \to M$ to be $\varphi^*_\alpha\colon \pi_1^{-1}(O_\alpha) \to O_\alpha \times F$ that act as $\varphi^*_\alpha((x, u)) = (x, \phi_\alpha(u))$. It follows that the transition function are related according to $\chi^*_{\alpha\beta}(x) = \chi_{\alpha\beta}(f(x))$.

An important theorem about pullbacked fibre bundles is the following: Let $E(B, \pi, F)$ be a fibre bundle, and f and g homotopic smooth maps from the smooth manifold M to the base space B. Then the pullbacked fibre bundles f^*E and g^*E are equivalent. For two smooth maps $f, g\colon M \to B$ we say that they are homotopic iff there exists a smooth map $F\colon [0, 1] \times M \to B$ such that $F(0, x) = f(x)$ and $F(1, x) = g(x)$ for every $x \in M$.

A local section of the fibre bundle $E(B, \pi, F)$ on the open subset $U \subseteq B$ is a smooth function $s\colon U \to E$ for which $U \ni x \mapsto s(x) \in E_x$. In words, to points in the base space it assigns points in the fibre above that point. Equivalently, we demand that the section satisfy $\pi \circ s = \mathrm{id}_U$. A global section is simply a local section defined over the whole base space, i.e., $U = B$. The set of local sections of $E \to B$ on $U \subseteq B$ we denote $\Gamma(U, E)$, and the set of global sections we denote $\Gamma(E)$.

Appendix E: Proofs of some identites

To prove the equivalence of definitions (31) and (32) of the connection 1-form $\mathcal{A}\colon TE \to \mathfrak{g}$, consider a local trivialization $(U_\alpha, \varphi_\alpha)$, a point p with $\varphi_\alpha(p) = (x, g)$, and a tangent vector $v \in T_pE$. To find the expression for $\mathcal{A}(v) = Z_p^{-1}\mathcal{A}'(v) = \xi$ in the local trivialization, we use their definitions:

$$\begin{aligned}
\mathcal{A}'_p(v) = Z_p(\xi) = \mathbf{X}_\xi(p) &= \frac{\mathrm{d}}{\mathrm{d}t}\tilde{R}(e^{t\xi}, p)\Big|_{t=0} \\
&= \frac{\mathrm{d}}{\mathrm{d}t}\varphi_\alpha^{-1}\Big(\varphi_\alpha(p)\cdot e^{t\xi}\Big)\Big|_{t=0} \\
&= \varphi_{\alpha *}^{-1}|_p \,\frac{\mathrm{d}}{\mathrm{d}t}\Big(\varphi_\alpha(p)\cdot e^{t\xi}\Big)\Big|_{t=0} \\
&= \varphi_{\alpha *}^{-1}|_p \,\frac{\mathrm{d}}{\mathrm{d}t}\Big(x, g\cdot e^{t\xi}\Big)\Big|_{t=0} \\
&= \varphi_{\alpha *}^{-1}|_p \left(x, \frac{\mathrm{d}}{\mathrm{d}t}L_g e^{t\xi}\big|_{t=0}\right) \\
&= \varphi_{\alpha *}^{-1}|_p \,(x, L_{g*}\xi)\,.
\end{aligned}$$

Inverting the last expression yields the desired result.

To prove equation (33), let us start from the right-hand side. Consider a point $p \in P$, a vector $v \in T_pP$ and a group element $g \in G$. Let us define $\xi := \mathrm{Ad}_{g^{-1}}\big(\mathcal{A}_p(v)\big)$. Then we have:

$$\mathrm{Ad}_g(\xi) = \mathcal{A}_p(v) = Z_p^{-1}\mathcal{A}'_p(v)\,,$$

which we can invert to get:

$$\begin{aligned}
\mathcal{A}'_p(v) = Z_p\big(\mathrm{Ad}_g(\xi)\big) &= \mathbf{X}_{\mathrm{Ad}_g(\xi)}(p) \\
&= \frac{\mathrm{d}}{\mathrm{d}t}\tilde{R}(e^{t\,\mathrm{Ad}_g(\xi)}, p)\Big|_{t=0} \\
&= \frac{\mathrm{d}}{\mathrm{d}t}\tilde{R}\big(I_g(e^{t\xi}), p\big)\Big|_{t=0} \\
&= \frac{\mathrm{d}}{\mathrm{d}t}\big(p\cdot g\cdot e^{t\xi}\cdot g^{-1}\big)\Big|_{t=0} \\
&= \frac{\mathrm{d}}{\mathrm{d}t}\tilde{R}_{g^{-1}}\big(\tilde{R}(e^{t\xi}, p\cdot g)\big)\Big|_{t=0} \\
&= \tilde{R}_{g^{-1}*}\frac{\mathrm{d}}{\mathrm{d}t}\big(\tilde{R}(e^{t\xi}, p\cdot g)\big)\Big|_{t=0} \\
&= \tilde{R}_{g^{-1}*}\mathbf{X}_\xi(p\cdot g) = \tilde{R}_{g^{-1}*}Z_{p\cdot g}(\xi)\,.
\end{aligned}$$

Moreover, since right translation acts along the fibres, the following is true:

$$\tilde{R}_{g*}\mathcal{A}'_p(v) = \mathcal{A}'_{p\cdot g}(\tilde{R}_{g*}v)\,.$$

Combining these two, we have $Z_{p\cdot g}(\xi) = \mathcal{A}'_{p\cdot g}(\tilde{R}_{g*}v)$, from which the equation follows.

To prove the relation (37) between two pushforwards of local sections $s\colon U \to P$ and $z\colon O \to P$, consider a curve $\gamma\colon \langle -1, 1\rangle \to B$ such that $\gamma(0) = x$ and $\dot\gamma(0) = v \in T_xB$. Using the definitions, we obtain:

$$\begin{aligned}
z_*(v) = \frac{\mathrm{d}}{\mathrm{d}t}z(\gamma_t)\Big|_{t=0} &= \frac{\mathrm{d}}{\mathrm{d}t}\big[s(\gamma_t)\cdot g_{sz}(\gamma_t)\big]\Big|_{t=0} \\
&= \frac{\mathrm{d}}{\mathrm{d}t}s(\gamma_t)\Big|_{t=0}\cdot g_{sz}(x) + s(x)\cdot\frac{\mathrm{d}}{\mathrm{d}t}g_{sz}(\gamma_t)\Big|_{t=0} \\
&= \tilde{R}_{g_{sz}(x)*}s_*(v) + z(x)\cdot g_{sz}^{-1}(x)\frac{\mathrm{d}}{\mathrm{d}t}g_{sz}(\gamma_t)\Big|_{t=0}\,.
\end{aligned}$$

In the second term we recognize:

$$\begin{aligned}
g_{sz}^{-1}(x)\frac{\mathrm{d}}{\mathrm{d}t}g_{sz}(\gamma_t)\Big|_{t=0} &= \frac{\mathrm{d}}{\mathrm{d}t}\Big[g_{sz}^{-1}(x)\frac{\mathrm{d}}{\mathrm{d}t}g_{sz}(\gamma_t)\Big]\Big|_{t=0} \\
&= g_{sz}^{-1}(x)\,\mathrm{d}g_{sz}\,(v) = \xi \in \mathfrak{g}\,,
\end{aligned}$$

which allows us to express the second term as:

$$\begin{aligned}
z(x)\cdot\xi = \frac{\mathrm{d}}{\mathrm{d}t}\tilde{R}\big(e^{t\xi}, z(x)\big)\Big|_{t=0} &= \mathbf{X}_\xi(z(x)) \\
&= Z_{z(x)}(\xi) = Z_{z(x)}g_{sz}^{-1}(x)\,\mathrm{d}g_{sz}\,(v)\,.
\end{aligned}$$

This proves the relation.