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A Brief Introduction to Topology and Differential Geometry in Condensed Matter Physics (Second Edition)

Antonio Sergio Teixeira Pires

Appendix A

Lie derivative

A.1 Integral curve

As we saw before, a vector field v on a smooth manifold M is an assignment to every point $p \in M$ of a vector $v(p) \in T_pM$. In a local coordinate system, we have (Curtis and Miller 1985)

$$v(p) = v^i(p)\frac{\partial}{\partial x^i}\bigg|_p. \tag{A.1}$$

Given two vector fields u and w, we can define a new vector field $[u, w]$, called the commutator of u and v, by

$$[u, w](f) = u[w(f)] - w[u(f)]. \tag{A.2}$$

In terms of components, we have

$$[u, w]^i = u^j\frac{\partial w^i}{\partial x^j} - w^j\frac{\partial u^i}{\partial x^j}. \tag{A.3}$$

A *curve* on a manifold M (as we saw before) is the smooth mapping

$$\sigma: I \to M,$$

where $I \subset \Re$, and if $t \in I$ we have $\sigma(t) \in M$. The 'curve' is defined to be the map itself, not the set of image points in M (see figure A1).

An *integral curve* σ of a vector field v is a curve in the manifold M whose tangent at $p = \sigma(t)$ is the vector $v(p)$ with $p \in M$. That is

$$\frac{d\sigma(t)}{dt} = v(\sigma(t)) = v^i(\sigma)\frac{\partial}{\partial x^i}. \tag{A.4}$$

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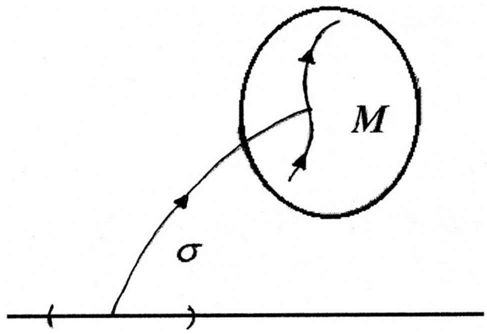

Figure A1. A curve in the manifold M.

Example. Let us consider in $\Re^2$ the vector field $v = y\partial/\partial x - (y + x)\partial/\partial y$ and the curve $\sigma(t) = (x(t), y(t))$. The integral curves of the vector field v satisfy the equation $\left(\frac{dx}{dt}, \frac{dy}{dt}\right) = v$. We have then $\frac{dx}{dt} = y$, $\frac{dy}{dt} = -(y + x)$, and so

$$\frac{dx^2}{dt^2} + \frac{dx}{dt} + x = 0,$$

which is the equation for the damped harmonic oscillator.

I will skip some theorems since they are too mathematical for our purposes. For any vector field v on the manifold M, there exists a smooth map $\sigma: \Re \times M \to M$ called the *flow* of v, written as $\sigma_t(p)$ with $t \in \Re$, and $p \in M$, such that $\sigma_0(p) = p$, $\sigma_t(\sigma_s(p)) = \sigma_{t+s}(p)$, and

$$\frac{d\sigma_t}{dt} = v(\sigma_t(p)). \tag{A.5}$$

The flow is a diffeomorphism with inverse σ_{-t}. Geometrically, σ_t sends each $p \in M$ to the point obtained by moving along the integral curve of v through p for a time t. Since σ_t is a map $M \to M$ we can think of the component σ_t^i with respect to the local coordinates x^i. Using (A.5) we get for small t

$$\sigma_t^i(p) = x^i(p) + tv^i(p) + O(t^2). \tag{A.6}$$

The set of points (t, p) with $t \in \Re$ and $p \in M$ is an open set of the space $\Re \times M$ and then a smooth manifold of dimension $n + 1$. Here I suppose that M is a compact manifold.

A.2 The Lie derivative

In general, geometric objects can be compared only if they are defined at the same point in the manifold. The geometric operation that provides the measure of the rate of change of a map is called the Lie derivative (Ebrain 2010, Friedman 2017, Harmark 2008). The simplest case is that of a function. The derivative $f\colon M \to \mathfrak{R}$ with respect to a vector field u, quantifies how much f changes along the flow of u. We use the difference between f in the point p and f in the translated point $\sigma_t(p)$:

$$£_u f(p) = \lim_{t\to 0}\left[\frac{f(\sigma_t(p)) - f(p)}{t}\right], \tag{A.7}$$

which becomes

$$£_u f(p) = \left.\frac{d}{dt}\right|_{t=0} f(\sigma_t(p)) = u(f)|_p. \tag{A.8}$$

Let us now turn to the case of vectors. But until we provide additional information, the concept of a vector field derivative is not well defined. We want to measure the rate of change of a vector field as we move from one point to another in the manifold, which means that we are implicitly comparing tangent vectors defined at different points p and q of M. There is no unique way to do this, since tangent vectors in p are in the tangent space T_pM and tangent vectors in q are in a different space T_qM. There are several ways to define mappings between these two spaces, but there is no unique or natural mapping. As we saw before, choosing a particular mapping between tangent spaces in the manifold imposes an additional structure called a connection. The derivative that uses a connection defined in M is the covariant derivative. The Lie derivative provides an alternative method, which does not require a connection, to derive vector fields and therefore apply in a general unstructured smooth manifold.

If u and v are vector fields in M, the Lie derivative (which gives the measure of the rate of change of v in the direction of u) can be defined as follows.

Let $q \in M$ be defined by $q = \sigma_t(p) \equiv p(t)$, and v a tangent vector $v(p) \in T_pM$.

Note that both vectors u and v are tangent vectors at p, but only u is tangent to the curve described by the point $p(t)$. Let M and N be smooth manifolds and f a mapping $f\colon M \to N$, with $p \in M$, $q \in N$. If c is a curve in M with $dc(0)/dt = u$, then $f \cdot c$ is a curve in N. We saw in chapter 3 that $Df\colon T_pM \to T_qN$ takes a tangent vector in M into a tangent vector in N. Now, if $M = N$, $f\colon M \to M$, with $f(p) = q$ where $p, q \in M$, takes a tangent vector at p into a tangent vector at q.

In figure A2, u is a tangent vector to the curve $p(t)$ (not shown in the figure), and v is the vector we want to calculate the variation along the curve. We know that σ_t takes the point p at $t = 0$ to the point $p(t) = q$. We have that $v(q) = v(\sigma_t(p))$ is the vector v at the point q.

We also know that $D\sigma_t\colon T_pM \to T_qN$ takes a tangent vector in p in the tangent vector in q and therefore, the inverse mapping $(D\sigma_t)^{-1}$ takes the tangent vector in q in the tangent vector in p (pulls back the vector). Note that $v(p)$ is tangent to a curve $\tilde{c}(t)$ that passes through p, but this curve is not the curve $p(t) = \sigma_t(p)$ in which u is tangent. The difference between $v(q)$ and $v(p)$ in the point p is then given by

$$\Delta = (D\sigma_t)^{-1}v(q) - v(p), \tag{A.9}$$

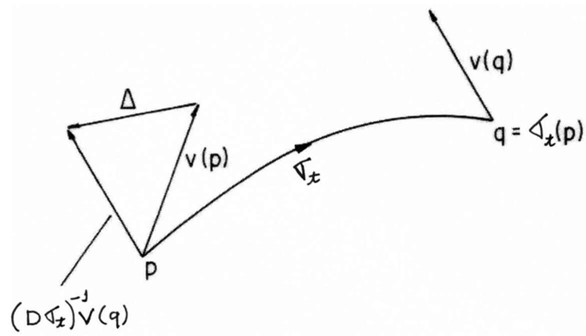

Figure A2. Lie derivative of a vector.

which leads to the following definition of the Lie derivative

$$£_u v(p) = \lim_{t=0} \frac{1}{t}[(D\sigma_t)^{-1} v(\sigma_t(p)) - v(p)], \tag{A.10}$$

or

$$£_u v(p) = \left.\frac{d}{dt}\right|_{t=0} (D\sigma_t)^{-1} \cdot v \cdot \sigma_t(p). \tag{A.11}$$

The derivative $£_u v(p)$ measures how $v(p)$ changes, compared with what would happen were it simply 'dragged along' by the vector field u. Writing the Lie derivative in terms of coordinates, it is easy to show that

$$£_u w = [u, w]. \tag{A.12}$$

The Lie derivative has the following properties

(a) $£_u(v + w) = £_u v + £_u w$
(b) $£_u(fv) = f£_u v + (£_u f)v$
(c) $£_{[v,u]} = [£_v, £_u]$.

The Lie derivative of a 1-form α can be obtained taking a vector field v and the function $f = \alpha(v)$. We have

$$£_u f = (£_u \alpha) \cdot v + \alpha \cdot £_u v, \tag{A.13}$$

which gives

$$(£_u \alpha) \cdot v = d(\alpha \cdot v)u - \alpha[u, v]. \tag{A.14}$$

The Lie derivative can be generalized to tensors. In particular, a Killing vector on a (pseudo-)Riemannian manifold M is a vector field u which has the property that Lie differentiation with respect to it annihilates the metric:

$$£_u g = 0. \tag{A.15}$$

A.3 Interior product

Let M be a manifold of dimension n, $\omega \in \Lambda^{k+1}(M)$ a $k+1$ form, and v a vector field. We define the interior product $i_v\colon \Lambda^{k+1}(M) \to \Lambda^k(M)$ by

$$i_v\omega(v_1, v_2, \dots, v_k) = \omega(v, v_1, \dots, v_k). \tag{A.16}$$

So $i_v\omega$ is a k-form. It can be shown that

(a) $di_v + i_v d = \pounds_v$.

(b) $[\pounds_v, i_u] = i_{[v,u]}$.

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Appendix B

Complex vector spaces

The definition of a vector space presented in chapter 1 can be extended to the complex case taking the scalars as complex numbers. The scalar product is now substituted by the Hermitian product (Groecheneg 2016, Kobayashi 1987).

Let V be a vector space over the complex numbers. A Hermitian product on V is a rule which to any pair of elements v, u of V associates a complex number, denoted $\langle v, u\rangle$, satisfying the following conditions:

(a) We have $\langle v, u\rangle = \overline{\langle u, v\rangle}$ for all $v, u \in V$ (the bar denotes complex conjugate).
(b) If, $u, v, w \in V$, then $\langle u, v + w\rangle = \langle u, v\rangle + \langle u, w\rangle$.
(c) If $\alpha \in \mathbb{C}$, then $\langle u, \alpha v\rangle = \alpha\langle u, v\rangle$, $\langle \alpha u, v\rangle = \bar{\alpha}\langle u, v\rangle$.

The Hermitian product is called *positive definite* if $\langle v, v\rangle \geqslant 0$ for all $v \in V$, and $\langle v, v\rangle > 0$ if $v \neq 0$.

B.1 Complex manifolds

At first, it seems that the definition of a complex manifold is similar to that of a smooth manifold, replacing open subsets of $\mathfrak{R}^n$ with open subsets of $\mathbb{C}^n$, and smooth functions by holomorphic functions. However, the complex analogous often yields more restrictions.

Let z denote any point of some neighborhood of a fixed point z_0, where the neighborhood is within the domain of definition of a function f. The derivative of f at z_0 is defined by the equation (Churchill 1960)

$$f'(z_0) = \lim_{\Delta z \to 0} \frac{f(z_0 + \Delta z) - f(z_0)}{\Delta z}, \tag{B.1}$$

where $\Delta z = z - z_0$.

We say the f is complex differentiable, or holomorphic, if and only if the limit exists for every $x \in U$ ($U \subset \mathbb{C}$). The derivative of a complex differentiable function is always continuous. Every holomorphic function is infinitely many times complex differentiable.

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Let M be a bounded compact n-dimensional manifold with a boundary ∂M. For every smooth $(n-1)$ form ω we have the Stoke's theorem

$$\int_M d\omega = \int_{\partial M} \omega. \tag{B.2}$$

The function $f\colon U \to \mathbb{C}$ (where $f(x, y) = u(x, y) + \mathrm{i}v(x, y)$) is holomorphic if and only if u and v are differentiable and satisfy the Cauchy–Riemann condition:

$$\frac{\partial u}{\partial x} = \frac{\partial v}{\partial y}, \qquad \frac{\partial v}{\partial x} = -\frac{\partial u}{\partial y}. \tag{B.3}$$

We introduce the complex 1-form $dz = dx + \mathrm{i}dy$, and define a second complex 1-form as $\omega = f(z)dz = (u + \mathrm{i}v)(dx + \mathrm{i}dy) = (udx - vdy) + \mathrm{i}(udy + vdx)$. Note that dz and $d\bar{z} = dx - \mathrm{i}dy$ are linearly independent.

A complex-valued function f, such that u and v are differentiable, satisfies the Cauchy–Riemann condition only if $\omega = f(z)dz$ satisfy $d\omega = 0$.

Proof:

$$\begin{gathered} d[(udx - vdy) + \mathrm{i}(udy + vdx)] \\ = \frac{\partial u}{\partial y}dy \wedge dx - \frac{\partial v}{\partial x}dx \wedge dy + \mathrm{i}\frac{\partial u}{\partial x}dx \wedge dy + i\frac{\partial v}{\partial y}dy \wedge dx. \end{gathered}$$

Using $dx \wedge dy = -dy \wedge dx$ we find

$$d\omega = \left[\left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x}\right) + \mathrm{i}\left(\frac{\partial u}{\partial x} - \frac{\partial v}{\partial y}\right)\right]dx \wedge dy. \tag{B.4}$$

So $d\omega = 0$ implies the vanishing of both the real and imaginary part, which corresponds to the Cauchy–Riemann condition.

Definition 1. Let X be a topological space together with an open covering $\{U_i\}$ with $i \in I$, and homeomorphisms: $\phi_i\colon U_i \to U'_i$, where $U'_i \subset \mathbb{C}^n$ is an open subset. If for every pair (i, j) the induced mapping

$$\phi_j \cdot \phi_i^{-1}\colon \phi_i(U_i \cap U_j) \to \phi_j(U_i \cap U_j), \tag{B.5}$$

is holomorphic, we say that X is endowed with the structure of a complex manifold of complex dimension n. The pair (U_i, ϕ_i) are called charts.

The covering $X = \cup_i U_i$ introduces a system of locally defined complex coordinates.

Definition 2. Let X be a continuous manifold and $f\colon X \to \mathbb{C}$ a continuous map. We say that f is holomorphic if, for every chart (U, ϕ) as above, the composition $f \cdot \phi^{-1}\colon U' \to \mathbb{C}$ is a holomorphic function on U'.

If X is a compact, connected, complex manifold, then every holomorphic function $f\colon X \to \mathbb{C}$ is constant. That implies that a compact complex manifold cannot be embedded into any $\mathbb{C}^n$.

We can think of a vector bundle $E \to X$ as a family of complex vector spaces over X. To each point $x \in X$ we associate a vector space $\pi^{-1}(X)$. The complex manifold E is the total space, X is the base, and π the structure map.

A *complex line bundle* L over a manifold M is a manifold L and a smooth mapping π: $L \to M$, such that (Murray 2016)

(1) Each fiber $\pi^{-1}(m) = L_m$ is a complex one-dimensional vector space.
(2) Every $m \in M$ has an open neighborhood $U \in M$ for which there is a diffeomorphism φ: $\pi^{-1}(U) \to U \times \mathbb{C}$ such that $\varphi(L_m) \in \{m\} \times \mathbb{C}$ for every m, and the map $\varphi|_{L_m}$: $L_m \to \{m\} \times \mathbb{C}$ is an isomorphism.

A *Hermitian manifold* is a complex manifold with a smoothly varying Hermitian inner product on each (holomorphic) tangent space. We can also define a Hermitian manifold as a real manifold with a Riemannian metric that preserves a complex structure.

The *Grassmannian* Gr(m, n), which is the space of m-dimensional subspaces of an n-dimensional complex vector space $\mathbb{C}^n$ (with $m \leqslant n$) is relevant to the classification of topological phases of condensed matter because it is associated with an n-dimensional quantum system with m occupied levels.

Let V be a real vector space. The complexification of V is defined by taking the tensor product of V with the complex numbers (thought of as a two-dimensional vector space over the real numbers):

$$V^C = V \otimes \mathbb{C}. \tag{B.6}$$

Every vector v in V^C can be written in the form

$$v = v_1 \otimes 1 + v_2 \otimes i, \tag{B.7}$$

where $v_1, v_2 \in V$. It is common to write: $v = v_1 + v_2$.

Let V be a vector space with dimension n over the complex numbers. If $\{e_n\}$ is a basis for V and $v \in V$ we can write $v = x_1 e_1 + x_2 e_2 + \cdots + x_n e_n$, where x_i are complex numbers. Writing $x_i = a_i + \mathrm{i}b_i$, where a_i and b_i are real numbers we have $v = a_1 e_1 + b_1 \mathrm{i}e_1 + \cdots + a_n e_n + b_n \mathrm{i}e_n$. Then $\{e_n, \mathrm{i}e_n\}$ is a basis for the underlying real vector space V_R of dimension $2n$.

If η is a complex vector bundle, then the underlying real bundle η_R has a canonical orientation.

Proof: Let V be a finite-dimensional complex vector space with basis $\{e_n\}$ over $\mathbb{C}$. As was demonstrated above, the set $\{e_n, \mathrm{i}e_n\}$ gives a real basis for V_R. This ordered basis determines the required orientation for V_R, since if $\{e'_n\}$ is another complex basis of V, then there is a $n \times n$ complex matrix A (with $\det A \neq 0$) which transforms the first basis into the second. This transformation does not alter the orientation of the real vector space, since A is the coordinate change matrix. Then the underlying $2n \times 2n$ real matrix A_R has: $\det A_R = |\det A|^2 > 0$. Hence A_R preserves the orientation of the underlying real vector space. We may apply this construction to each fiber of η to obtain the required orientation of η_R.

By the above discussion, we conclude that every complex manifold is oriented since an orientation of the tangent bundle of a manifold induces an orientation of the manifold itself.

Let us consider a closed curve $\gamma: S^1 \to \mathbb{C}\backslash\{0\}$ in the complex plane without the zero. The winding number of γ can be expressed as the complex integral

$$w[\gamma] = \deg[\lambda] = \frac{1}{2\pi i}\int_\gamma \frac{dz}{z} = \frac{1}{2\pi i}\int_\lambda d\log z, \tag{B.8}$$

and $w[\gamma] \in Z$ is an integer.

B.2 Complex projective space

A complex projective space CP^n ($\mathbb{C}$) is the set of lines in $\mathbb{C}^{n+1}$ passing through the origin. If $z = (z_0, \ldots, z_n) \neq 0$, the z determines the same line if $z = cz'$ for some complex $c \neq 0$, and they are called equivalent. CP^n ($\mathbb{C}$) is a complex manifold. It can be shown that CP^1 is diffeomorphic to the sphere S^2.

B.3 Hopf bundle

The Hopf bundle describes a 3-sphere in terms of circles and ordinary spheres. Hopf found a many-to-one continuous map from the 3-sphere onto the 2-sphere such that each distinct point of the 2-sphere comes from a distinct circle of the 3-sphere (Penrose 2007).

The unit 3-sphere $x_1^2 + x_2^2 + x_3^2 + x_4^2 = 1$ in $\mathfrak{R}^4$ can be thought of as a 3-sphere in $\mathbb{C}^2$, defined by the equation $|w|^2 + |z|^2 = 1$, where $w = x_1 + ix_2$, $z = x_3 + ix_4$. Let us consider now the space CP^1 of complex straight lines in $\mathbb{C}^2$ passing through the origin. Each line is given by an equation of the form $aw + bz = 0$, where a and b are complex numbers (not both zero). This line is a copy of a complex plane, and it meets S^3 in a circle S^1, which we can think of as a unit circle in that plane. These circles are the fibers of the bundle. The different lines can meet only at the origin, so no two distinct S^1s can have a point in common. Thus, this family of S^1s constitutes fibers giving S^3 a bundle structure. We can multiply a and b by the same non-zero complex number and get the same line: it is the ratio a/b that distinguishes one line from another. The space of such ratios is a Riemann sphere S^2, which we identify as the base space of the bundle. Thus the 3-sphere is realized as a disjoint union of circular fibers. The Hopf bundle is the simplest non-trivial vector bundle over the sphere S^2.

If we write $S^2 = \{(x, y, z) \in \mathfrak{R}^3, x^2 + y^2 + z^2 = 1\}$,

$$S^3 = \{(a, b, c, d) \in \mathfrak{R}_4, a^2 + b^2 + c^2 + d^2 = 1\},$$

the Hopf map $\pi: S^3 \to S^2$ is given by

$$\pi(a, b, c, d) = [(a^2 + b^2 - c^2 - d^2), 2(bc + ad), 2(bd - ac)i]. \tag{B.9}$$

Since $\pi_3(S^2) = \mathbb{Z}$, there is an associated integer called the Hopf invariant. This invariant cannot be the mapping degree since the domain and target spaces have different dimensions. We can define the mapping as follows. Let ω denote the area 2-form on the target S^2 and let $f = \vec{n}^*\omega$ be its pull-back under $\vec{n}$ to the domain S^3 (here $\vec{n}$ is a three-dimensional unit vector). Since ω is closed, f is also closed. The triviality of the second cohomology group of 3-spheres $H^2(S^3) = 0$ demands its pull-back to be an exact 2-form, which we write as $f = da$. The Hopf invariant is then given by integrating the Chern–Simons 3-form over S^3

$$W = \frac{1}{4\pi^2}\int_{S^3} f \wedge a. \tag{B.10}$$

This integral is independent of the choice of a, because if $a \to a + \mathrm{d}\alpha$, we have

$$\Delta W = \frac{1}{4\pi^2}\int_{S^3} (d(f\alpha) - (df)\alpha) = 0, \tag{B.11}$$

because $df = 0$, and by Stoke's theorem, the integral of $d(f\alpha)$ is zero over a closed three-manifold.

If we consider a two-band insulator in three dimensions and take the Brillouin zone as a sphere S^3, we can use the same Hamiltonian used in two dimensions and from the mapping $\pi_3(S^2) = \mathbb{Z}$ conclude that there are many different non-trivial phases. However, by adding a few trivial bands and using the K-theory it can be shown that the topological phases disappear (Thiang 2017).

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Appendix C

Fubini–Study metric and quaternions

C.1 Fubini–Study metric

Let us consider a Hamiltonian $H(\lambda)$ that depends smoothly on the set of parameters $\lambda = (\lambda_1, \ldots, \lambda_N)$ (Cheng 2013). If $\psi(\lambda)$ is a parameter-dependent wave function, we can try to define a quantum distance upon an infinitesimal variation of the parameter λ by

$$\begin{aligned} ds^2 = \|\psi(\lambda + d\lambda) - \psi(\lambda)\|^2 = \langle\delta\psi|\delta\psi\rangle = \left\langle\partial_\mu\psi\middle|\partial_\nu\psi\right\rangle d\lambda^\mu d\lambda^\nu \\ = (\gamma_{\mu\nu} + \mathrm{i}\sigma_{\mu\nu})d\lambda^\mu d\lambda^\nu, \end{aligned} \tag{C.1}$$

where $\gamma_{\mu\nu}$ is the real and $\sigma_{\mu\nu}$ the imaginary parts of ds^2. Using the property that the inner product is Hermitian, we have

$$\gamma_{\mu\nu} + \mathrm{i}\sigma_{\mu\nu} = \gamma_{\nu\mu} - \mathrm{i}\sigma_{\mu\nu}, \tag{C.2}$$

which gives $\gamma_{\mu\nu} = \gamma_{\nu\mu}$, and $\sigma_{\mu\nu} = -\sigma_{\nu\mu}$. Therefore $\sigma_{\mu\nu}d\lambda^\mu d\lambda^\nu$ vanishes due to the antisymmetry of $\sigma_{\mu\nu}$ and symmetry of $d\lambda^\mu d\lambda^\nu$. We can then write

$$ds^2 = \gamma_{\mu\nu}d\lambda^\mu d\lambda^\nu. \tag{C.3}$$

However, the above expression is not gauge-invariant, as we can see by taking

$$|\psi'(\lambda)\rangle = \mathrm{e}^{\mathrm{i}\alpha(\lambda)}\,|\psi(\lambda)\rangle, \tag{C.4}$$

and defining

$$\left\langle\partial_\mu\psi'\middle|\partial_\nu\psi'\right\rangle = \gamma'_{\mu\nu} + \mathrm{i}\sigma'_{\mu\nu}. \tag{C.5}$$

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We find

$$\gamma'_{\mu\nu} = \gamma_{\mu\nu} - \beta_\mu \partial_\nu \alpha - \beta_\nu \partial_\mu \alpha + \partial_\mu \alpha \partial_\nu \alpha, \qquad \sigma'_{\mu\nu} = \sigma_{\mu\nu}, \tag{C.6}$$

where $\beta_\mu(\lambda) = \mathrm{i}\langle\psi(\lambda)|\partial_\mu\psi(\lambda)\rangle$ is the Berry connection, which is purely real due to the normalization $\langle\psi(\lambda)|\psi(\lambda)\rangle = 1$. The Berry connection upon the above gauge transformation changes as $\beta'_\mu = \beta_\mu + \partial_\mu\alpha$. We define a gauge-invariant metric using the following expression

$$g_{\mu\nu} = \gamma_{\mu\nu} - \beta_\mu(\lambda)\beta_\nu(\lambda). \tag{C.7}$$

It is easy to show that under the gauge transformation we get $g'_{\mu\nu}(\lambda) = g_{\mu\nu}(\lambda)$.

We can also verify that the covariant derivative

$$|D_\mu\psi\rangle = |\partial_\mu\psi\rangle - |\psi\rangle\langle\psi|\partial_\mu\psi\rangle, \tag{C.8}$$

transforms as $|\psi\rangle$. The last term projects out parts of $|\partial_\mu\psi\rangle$ not orthogonal to $|\psi\rangle$.

The Fubini–Study metric is defined as

$$Q_{\mu\nu}(\lambda) = \left\langle \partial_\mu\psi(\lambda) \middle| \partial_\nu\psi(\lambda) \right\rangle - \left\langle \partial_\mu\psi(\lambda) \middle| \psi(\lambda) \right\rangle \left\langle \psi(\lambda) \middle| \partial_\nu\psi(\lambda) \right\rangle. \tag{C.9}$$

We define $g_{\mu\nu} = \mathrm{Re}\, Q_{\mu\nu}$, $\sigma_{\mu\nu} = \mathrm{Im} Q_{\mu\nu}$.

Taking the inner product of $|\psi(\lambda)\rangle$ and $|\psi(\lambda + \mathrm{d}\lambda)\rangle$, and expanding in a Taylor series we obtain

$$\langle\psi(\lambda)|\psi(\lambda + d\lambda)\rangle = 1 + \mathrm{i}\beta_\mu(\lambda)d\lambda^\mu + \frac{1}{2}\left\langle \psi(\lambda) \middle| \partial_\mu\partial_\nu\psi(\lambda) \right\rangle d\lambda^\mu d\lambda^\nu + \cdots \tag{C.10}$$

Using the fact that $\langle\psi|\partial\psi\rangle$ is pure imaginary we find that $\langle\partial_\mu\psi|\partial_\nu\psi\rangle + \langle\psi|\partial_\mu\partial_\nu\psi\rangle$ is also purely imaginary. We then get

$$\mathrm{Re}\left\langle \psi \middle| \partial_\mu\partial_\nu\psi \right\rangle = -\mathrm{Re}\left\langle \partial_\mu\psi \middle| \partial_\nu\psi \right\rangle = -\gamma_{\mu\nu}. \tag{C.11}$$

Equation (C.10) can then be written

$$\begin{aligned} |\langle\psi(\lambda)|\psi(\lambda + d\lambda)\rangle| &= 1 - \frac{1}{2}(\gamma_{\mu\nu}(\lambda) - \beta_\mu(\lambda))d\lambda^\mu d\lambda^\nu \\ &= 1 - \frac{1}{2}g_{\mu\nu}(\lambda)d\lambda^\mu d\lambda^\nu. \end{aligned} \tag{C.12}$$

The quantum distance between quantum states labeled by λ_I and λ_F can be written as

$$|\langle\psi(\lambda_F)|\psi(\lambda_1)\rangle| = 1 - \frac{1}{2}\int_{\lambda_I}^{\lambda_F} g_{\mu\nu}(\lambda)d\lambda^\mu d\lambda^\nu \tag{C.13}$$

The last term is called geometric quantum distance.

As an example, let us consider a two-level quantum system living in C^2, with a wave function

$$\psi(x) = \begin{pmatrix} \cos(\theta/2)\mathrm{e}^{\mathrm{i}\varphi} \\ \sin(\theta/2) \end{pmatrix}. \tag{C.14}$$

We have

$$\left\langle \psi \middle| \partial_\varphi \psi \right\rangle = \mathrm{i}\cos^2(\theta/2), \quad \left\langle \psi \middle| \partial_\theta \psi \right\rangle = 0, \tag{C.15}$$

$$\left\langle \partial_\varphi \psi \middle| \partial_\varphi \psi \right\rangle = \cos^2(\theta/2), \quad \left\langle \partial_\varphi \psi \middle| \partial_\theta \psi \right\rangle = -\mathrm{i}\frac{1}{4}\sin\theta. \tag{C.16}$$

$$\left\langle \partial_\theta \psi \middle| \partial_\theta \psi \right\rangle = 1/4. \tag{C.17}$$

The components of the Fubini–Study metric are then given by

$$g_{\theta\theta} = \frac{1}{4}, \qquad g_{\theta\varphi} = 0, \qquad g_{\varphi\varphi} = \frac{1}{4}\sin^2\theta. \tag{C.18}$$

We see that the metric agrees with the standard metric on a sphere of radius ¼.

The field associated to the connection β_μ, is given by

$$\mathfrak{F}_{\mu\nu} = \partial_\mu \beta_\nu - \partial_\nu \beta_\mu = \mathrm{i}\big(\partial_\mu \langle \psi | \partial_\nu \psi \rangle - \partial_\nu \langle \psi | \partial_\mu \psi \rangle\big). \tag{C.19}$$

From the normalization condition $\langle \psi | \psi \rangle = 1$, we get

$$\left\langle \psi \middle| \partial_\mu \psi \right\rangle = -\left\langle \partial_\mu \psi \middle| \psi \right\rangle. \tag{C.20}$$

Using (C.20) in (C.19) and comparing with (C.9), we find

$$\mathfrak{F}_{\mu\nu} = \mathrm{i}(Q_{\mu\nu} - Q_{\nu\mu}) = -2\mathrm{Im}Q_{\mu\nu} = -2\sigma_{\mu\nu}. \tag{C.21}$$

We can also write

$$Q_{\mu\nu} = g_{\mu\nu} - \frac{\mathrm{i}}{2}\mathfrak{F}_{\mu\nu}. \tag{C.22}$$

Suppose now that there is a large gap between the ground state $|\phi_0(\lambda)\rangle$ and the first excited state, such that transitions can be ignored. We have

$$H(\lambda)|\phi_0(\lambda)\rangle = E_0(\lambda)|\phi_0(\lambda)\rangle, \tag{C.23}$$

with

$$\left\langle \phi_n(\lambda) \middle| \phi_0(\lambda) \right\rangle = \delta_{n0}. \tag{C.24}$$

Taking the derivative of (C.23), we find

$$(\partial_\mu H)|\phi_0\rangle + H\partial_\mu|\phi_0\rangle = E_0\partial_\mu|\phi_0\rangle. \tag{C.25}$$

Using (C.20), we find

$$\begin{aligned} \langle \phi_n | \phi_0 \rangle &= \frac{\langle \phi_n | \partial_\mu H | \phi_0 \rangle}{E_0 - E_n}, \quad \text{if } n \neq 0, \\ \langle \phi_0 | \partial_\mu H | \phi_0 \rangle &= \partial_\mu E_0. \end{aligned} \tag{C.26}$$

On the ground state, we have

$$\begin{aligned} Q_{\mu\nu} &= \langle \partial_\mu \phi_0 | (1 - |\phi_0\rangle\langle\phi_0|) | \partial_\mu \phi_0 \rangle = \sum_{n \neq 0} \langle \partial_\mu \phi_0 | \phi_n \rangle \langle \phi_n | \partial_\nu \phi_0 \rangle \\ &= \sum_{n \neq 0} \frac{\langle \phi_0 | \partial_\mu H | \phi_n \rangle \langle \phi_n | \partial_\nu H | \phi_0 \rangle}{(E_0 - E_n)^2}. \end{aligned} \tag{C.27}$$

Note: Sometimes, the distance between two states $|\psi\rangle$ and $|\phi\rangle$ (not normalized) are presented in the literature as

$$\gamma(\psi, \phi) = \arccos \sqrt{\frac{\langle \psi | \phi \rangle \langle \phi | \psi \rangle}{\langle \psi | \psi \rangle \langle \phi | \phi \rangle}}. \tag{C.28}$$

Taking $\phi = \psi + \delta\psi$, and using the expansion $\cos\sqrt{\mathrm{d}s^2} = 1 - \frac{1}{2}\mathrm{d}s^2$, we get the former result for the Fubini–Study metric. For a study relating the Fubini–Study metric to the topological invariant of generic Dirac Hamiltonians, see Mera and Goldman (2021).

C.2 Quaternions

Quaternions have been used in the study of Landau levels in topological insulators in three dimensions (Li and Wu 2013). It is appropriate, therefore, that I comment on this subject briefly here.

In the 19th century, the Irish mathematician William Rowan Hamilton (1805–65) generalized the complex numbers to a four-dimensional space, with the imaginary basis-vectors extended from one (i) to three (i, j, k) with the following property (Penrose 2007)

$$\begin{aligned} & i^2 = j^2 = k^2 = ijk = -1 \\ & ij = -ji = k, \quad jk = -kj = i, \quad ki = -ik = j \end{aligned} \tag{C.29}$$

A quaternion q can be written as

$$q = q_0 + iq_1 + jq_2 + kq_3 \tag{C.30}$$

where q_i are real numbers.

Quaternions satisfy the commutative and associative laws of addition and the distributive laws of multiplication over addition, namely

$$\begin{aligned} & a + b = b + a, \qquad a + (b + c) = (a + b) + c \\ & a(bc) = (ab)c, \qquad a(b + c) = ab + ac, \qquad (a + b)c = ac + bc \end{aligned}$$

together with the existence of additive and multiplicative ‘identity element’ 0, and 1, such that

$$a + 0 = a, \quad 1a = a1 = a$$

we define $q^* = q_0 - iq_1 - jq_2 - kq_3$ and the norm of q is given by

$$|q| = \sqrt{qq^*} = \sqrt{q_0^2 + q_1^2 + q_2^2 + q_3^2}. \tag{C.31}$$

For each non-zero quaternion q, there is an inverse q^{-1} that satisfies

$$q^{-1}q = qq^{-1} = 1.$$

We have

$$q^{-1} = q^*(qq^*)^{-1}$$

The real number qq^* cannot vanish unless $q = 0$.

If $q_1 = (x_1, y_1, z_1, w_1)$ and $q_2 = (x_2, y_2, z_2, w_2)$, we have

$$\begin{aligned} q_1q_2 = {} & x_1x_2 - y_1y_2 - z_1z_2 - w_1w_2 + x_1y_2 + y_1x_2 + z_1w_2 - w_1z_2 \\ & + x_1z_2 + z_1x_2 + w_1y_2 - y_1w_2 + x_1w_2 + w_1x_2 + y_1z_2 - z_1y_2 \end{aligned}$$

We can define vector spaces over quaternions, however, there is no satisfactory quaternionic analogous of the notion of a holomorphic function.

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