CeFEMA Informal Discussion: Geometric phases in Quantum Mechanics

B. Mera

Instituto Superior Técnico
CeFEMA and Physics of Information Group

11th November, 2016

outline

Berry Phase from a geometric point of view

Berry Phase from “Parametric” Hamiltonians

“Parametric” Hamiltonians

If we have a quantum mechanical system described by a Hamiltonian depending (smoothly) on some parameters living on a space X (usually a manifold), say $H(x)$, then, we can consider the eigenvalue problem,

$$H(x) \cdot v = \lambda \cdot v$$

Solving $\det(H(x) - \lambda I) = 0$, we find the collection of “bands” $\{\lambda_i(x) : x \in X\}_{i \in I}$.
For each $i \in I$, we can form the eigenspace $E_x^i = \{v : H(x) \cdot v = \lambda_i(x) \cdot v\}$.

Eigenvector bundles

In general, there is no guarantee, that $\dim E_x^i$ will be constant as a function of $x \in X$. Usually, a gap condition provides this.Let us assume this and focus now on one of the bands. For commodity we drop the index i.
Locally we can now solve for $H(x) \cdot v = \lambda(x) \cdot v$ and, by smoothness, we can extend a solution at a point $x \in X$ to an open neighbourhood $U \subset X$. This means that, over U, the set $E|_U = \{(x, v) : x \in U,\ v \in E_x\}$ is, topologically, a Cartesian product $U \times \mathbb{C}^k$, where $k = \dim E_x$. The set $E = \{(x, v) : x \in X,\ v \in E_x\}$, equipped with the projection $\pi : E \ni (x, v) \mapsto x \in X$, is what mathematicians call a vector bundle.

“Wave-functions” as sections

The space E is contained in $X \times V$, where V is the Hilbert space of the Quantum Mechanical problem. The space $X \times V$, equipped with the projection onto the first factor, is a trivial vector bundle since it is globally a Cartesian product. In particular, we know how to take derivatives of smooth “wave-functions” $\psi : x \mapsto \psi(x) \in V$. Mathematically, these wave-functions, seen as maps $s_\psi : X \to X \times V$, are called (cross-)sections of the vector bundle.

Berry connection

Essentially, the notion of connection provides a way to take derivatives, along tangent vectors of X, of sections of E. The Berry connection is a natural choice, given the fact that we have an Hermitian inner product on V to start with. We can hence define, for each x, an orthogonal projection $P_x : V \to E_x$. Now for any section of E seen as a section of $X \times V$, the projection of the derivative along a tangent vector is always in E. This defines a covariant derivative ∇ on E.

Local form of the Berry connection

Given a local o.n. basis for E over an open set $U \subset X$, $\{v_1(x), ..., v_k(x)\}$, then a section of E is written as,

$$\psi(x) = \sum_{i=1}^{k} a^i(x) v_i(x).$$

The derivative of ψ seen as a section of $X \times V$, would be

$$d\psi(x) = \sum_{i=1}^{k} \left(da^i(x) v_i(x) + a^i(x) dv_i(x) \right)$$

Local form of the Berry connection (cont.)

Because of the second term, we could leave the space E_x. But now,

$$
\begin{aligned}
\nabla\psi(x) &:= P_x(d\psi(x)) \\
&= \sum_{i=1}^{k} \left(da^i(x) v_i(x) + \sum_{j=1}^{k} \langle v_j(x), dv_i(x) \rangle a^i(x) v_j(x) \right) \\
&= \sum_{i=1}^{k} \left(da^i(x) + \sum_{j=1}^{k} \langle v_i(x), dv_j(x) \rangle a^j(x) \right) v_i(x).
\end{aligned}
$$

Berry connection coefficients

From the local expression,

$$\nabla\psi(x) = \sum_{i=1}^{k}\left(da^i(x) + \sum_{j=1}^{k}\langle v_i(x), dv_j(x)\rangle a^j(x)\right) v_i(x),$$

we can identify the local connection coefficients,

$$\omega^i_j(x) = \langle v_i(x), dv_j(x)\rangle,$$

which, clearly, satisfy,

$$\omega^i_j(x) = -\bar{\omega}^j_i(x).$$

Equivalently, the matrix of $1-$forms $\omega(x) = [\omega^i_j(x)]_{1\leq i,j\leq k}$ is skew-Hermitian, hence lives in the Lie algebra of the unitary group $\mathrm{U}(k)$ – $\mathfrak{u}(k)$.

Parallel Transport

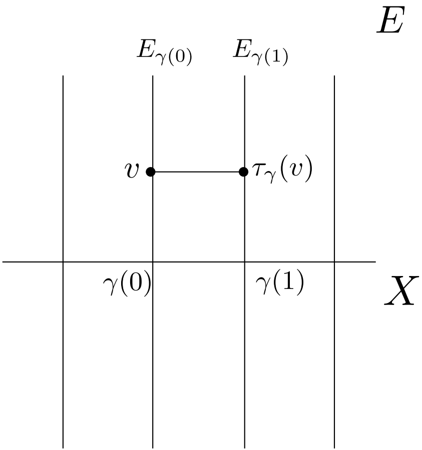
Consider a (smooth) curve in the space of parameters X, namely $\gamma : [0,1] \to X$ with $\gamma([0,1]) \subset U \subset X$. The parallel transport of a vector $v \in E_{\gamma(0)}$ along γ, $\tau_\gamma(v) \in E_{\gamma(1)}$, is simply the value at $\gamma(1)$ of the unique section s_v (defined on $\gamma([0,1])$, with $s_v(\gamma(0)) = v$, that is covariantly conserved along γ,

$$\nabla_{\dot\gamma}(s_v) = 0, \text{ over } \gamma([0,1]).$$

Writing $s_v(\gamma(t)) = \sum_i a^i(t) v_i(\gamma(t))$, this amounts to solving the ODE,

$$\frac{da^i}{dt}(t) + \sum_j \omega^i_j(\dot\gamma) a^j(t) = 0,$$
$$v = \sum_i a^i(0) v_i(\gamma(0)).$$

Illustration of the concept of parallel transport



Parallel Transport (cont.)

If we write $a(1) = [a^1(1) \ldots a^k(1)]^t$ as a column vector, the formal solution is

$$a(1) = U \cdot a(0),$$

with

$$U = T \exp(-\int_0^1 dt \; \omega(\dot{\gamma}))$$

When $\dim E = 1$, then, $\omega = \langle v, dv \rangle \equiv -i\mathcal{A}$, and we write,

$$U = \exp(i \int_0^1 dt \; \mathcal{A}(\dot{\gamma})),$$

where the local 1-form $\mathcal{A}$ is what is usually called the Berry gauge field.

Berry Phase from the U(1) ambiguity of Quantum Mechanics

We would now like to see the Berry connection from a slightly different perspective. In quantum mechanics, there is a phase ambiguity in defining the wave-function. Namely, we consider normalized vectors in the Hilbert space, i.e. ψ s.t. $||\psi||^2 = 1$, and we say that ψ and $\psi \cdot e^{i\alpha}$ correspond to the same state. Therefore the state is not a vector, but a one-dimensional subspace, a "ray", of the vector space.

For simplicity, let us consider the vector space $\mathbb{C}^n$. A state is then represented by a normalized vector $\psi \in S^{2n-1} \subset \mathbb{C}^n$. The state itself is an equivalence class $[\psi] = \{\psi \cdot e^{i\alpha} : e^{i\alpha} \in \mathrm{U}(1)\}$. Now if I take a curve $\psi(t)$ of such vectors, there are directions which are tangent to the fiber, i.e., directions which change the phase but not the state (vertical vectors), and directions which change the state (horizontal vectors). For a given vector ψ, the vertical vectors are easily seen to be of the form $\psi \cdot i\alpha$ with $\alpha \in \mathbb{R}$, hence

$$V_\psi = \{\psi \cdot i\alpha : \alpha \in \mathbb{R}\} \subset T_\psi S^{2n-1} \subset T_\psi \mathbb{C}^n$$

In general, there is no canonical way to identify the horizontal vectors because there are many vector space complements of V_ψ in $T_\psi S^{2n-1}$. However, since we are given an inner product (the real part of the Hermitian inner product in $\mathbb{C}^n$) in the vector space there is a canonical choice, namely the orthogonal complement.

Explicitly,

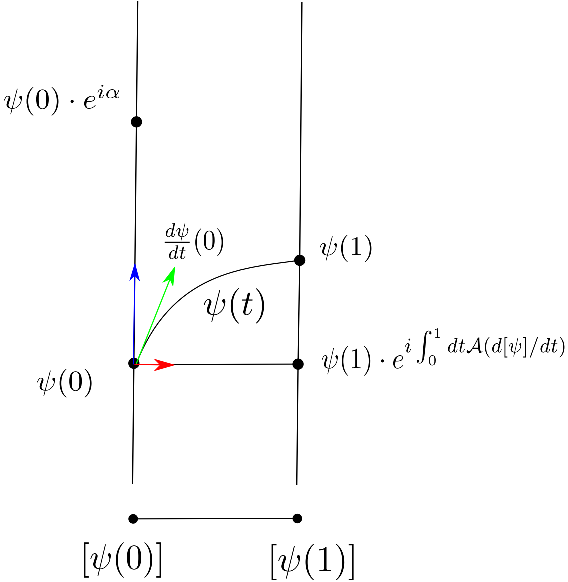
$$H_\psi = \{v \in T_\psi S^{2n-1} : \mathrm{Im}\langle v, \psi\rangle = 0 \Leftrightarrow \langle v, \psi\rangle = 0\}.$$

Next, consider a curve of normalized vectors $\psi(t)$, $t \in [0,1]$, which projects to a curve of states $[\psi(t)]$, $t \in [0,1]$. We want to consider a lift of the projected curve such that the velocity is always horizontal. This gives a notion of horizontal lift. The relation between the original curve $\psi(t)$ and the horizontal lift $\widetilde{\psi}(t)$ will be a phase factor:

$$\widetilde{\psi}(t) = \psi(t) \cdot e^{i\alpha(t)}.$$

In particular, we can choose that $\tilde{\psi}(0) = \psi(0)$, so that $e^{i\alpha(0)} = 1$.

Illustration of the concept of horizontal lift



The horizontality condition then yields,

$$\langle \frac{d\tilde{\psi}}{dt}, \tilde{\psi} \rangle = 0,$$

which gives,

$$i \frac{d\alpha}{dt} = \langle \psi, \frac{d\psi}{dt} \rangle,$$

hence,

$$\tilde{\psi}(t) = \psi(t) \cdot e^{i \int_0^1 dt \langle \psi, \frac{d\psi}{dt} \rangle},$$

which has exactly the same form as the Berry geometric phase encountered previously. In fact, the two constructions can be shown to be equivalent, but I rather skip this step, since the audience wants to know about the Uhlmann phase.

Uhlmann Phase

When we consider the general framework of mixed states, the state $[\psi]$ gets replace by the orthogonal projector P_ψ, commonly denoted by $|\psi\rangle\langle\psi|$. Notice that the projector P_ψ does not have the phase ambiguity. More generally, we can consider arbitrary density matrices ρ. What is the analogue of the vector ψ in this case?

For simplicity consider that the space of pure states is again $\mathbb{C}^n$. Then, if ρ has rank $= k \leq n$, there exists $w \in \mathbb{C}^{n \times k}$ (called an *amplitude* for ρ) such that,

$$\rho = ww^*,$$

essentially w is a matrix whose columns are the eigenvectors of ρ, with appropriate weights concerning the eigenvalues of ρ. The choice of w is not unique. Essentially, if we take $w \mapsto w \cdot U$, $U \in \mathrm{U}(k)$ the expression is left invariant. Hence, for fixed rank k, there is a $\mathrm{U}(k)$ ambiguity. Notice that when $k = 1$, $w \in \mathbb{C}^n$ and the normalization condition $\mathrm{tr}\rho = 1$ implies $||w||^2 = 1$.

Next, we wish to identity the analogue of the Berry phase in this case – the Uhlmann phase.
The vertical subspace of the tangent space at w of the space of amplitudes is easily identified to be

$$V_w = \{w \cdot X : X \in \mathfrak{u}(k)\}$$

The space of amplitudes for density matrices of rank k is contained in the vector space $\mathbb{C}^{n \times k}$, where we have the Hermitian structure

$$\langle w_1, w_2 \rangle = \mathrm{tr}(w_1^* w_2).$$

and a real inner product (the real part of the above expression).
With this, we can identify, uniquely, the horizontal subspace at w

$$\begin{aligned} H_w &= \{v : \mathrm{Re}\ \mathrm{tr}(v^* w X) = 0, \text{ for any } X \in \mathfrak{u}(k)\} \\ &= \{v : v^* w = w^* v\} \end{aligned}$$

Now if we have a curve of density matrices of fixed rank k, $\rho(t)$, the criterion for a lift $w(t)$ to be horizontal is given by

$$\frac{dw^*}{dt}w - w^*\frac{dw}{dt} = 0.$$

From which we can obtain the local form of the Uhlmann connection.

Of particular importance is the case of a full rank density matrix ρ (for e.g. a Gibbs ensemble at finite T). In this case, there is a canonical lift for ρ, namely,

$$w = \sqrt{\rho}.$$

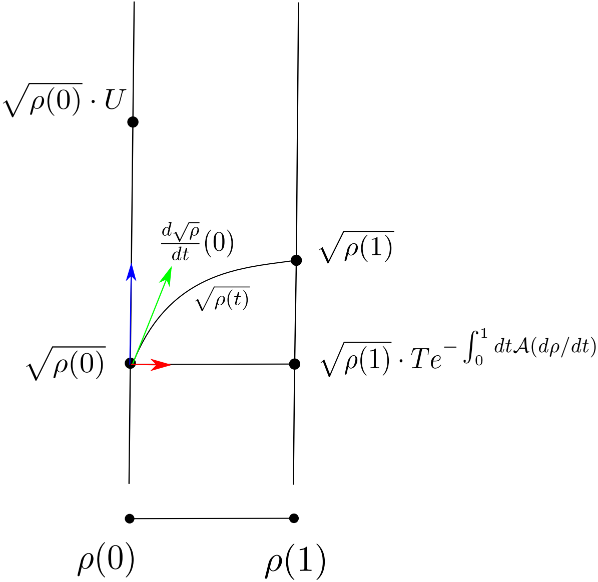
In topological terms, this means that the bundle of amplitudes over the space of states is trivial (there exists a global section).
The Uhlmann connection is, in this particular case, represented by a globally defined $\mathfrak{u}(n)$-valued one-form.

The horizontality condition yields, for a lift $w(t) = \sqrt{\rho}(t) \cdot U(t)$, of a curve of states $\rho(t)$, $t \in [0,1]$, reads

$$[\sqrt{\rho}, \frac{d\sqrt{\rho}}{dt}] - \{U \cdot \frac{dU^*}{dt}, \rho\} = 0.$$

And $U \cdot dU^*/dt = -dU/dt \cdot U^* \equiv \mathcal{A}(d\rho/dt)$ is the Uhlmann connection evaluated at the tangent vector on the space of states $d\rho/dt$.

Parallel transport of amplitudes



The Uhlmann phase is strongly connected with the quantum information concept of Fidelity. Perhaps some other time I can explain this relationship.