Quantum splines

David Meier, joint work with Dorje Brody and Darryl Holm

11 July

Spin-off from work with Christopher Burnett, François Gay-Balmaz, Darryl Holm, Tudor Ratiu and François-Xavier Vialard

$\longrightarrow$ **Minisymposium Wednesday 18 July**

Quantum mechanics

- **Hilbert space** $\mathcal{H}$. Finite-dimensional Hilbert space $\mathcal{H} = \mathbb{C}^{n+1} \leftrightsquigarrow$ Systems of quantum mechanical **angular momentum/spin**
- **Notation:** Denote elements of $\mathcal{H}$ by $|\psi\rangle$. Hermitian conjugate is denoted $\langle\psi|$.
- Quantum **state space** given by complex projective space $\boxed{\mathbb{CP}^n = (\mathbb{C}^{n+1} - \{\mathbf{0}\})/\mathbb{C}}$
  $\leftrightsquigarrow$ **Normalization:** probabilistic nature of quantum mechanics.
  Phase invariance: experiments invariant wrt complex phase.
- **Schrödinger equation** describes evolution of state $|\psi\rangle$,

  $$\boxed{\partial_t|\psi_t\rangle = -\mathrm{i}H|\psi_t\rangle,}$$

  where the **Hamiltonian** H is a Hermitian (self-adjoint) matrix assumed trace-free. Therefore $-iH \in \mathfrak{su}(n+1)$, skew-Hermitian & trace-free.
- Alternative formulation of Schrödinger equation: State evolution $\boxed{|\psi_t\rangle = U(t)|\psi_0\rangle}$ with $U(t)$ a curve on the Lie group $SU(n+1)$ of **special unitary matrices**, satisfying

  $$\boxed{\dot{U} = -\mathrm{i}HU, \quad U(0) = \mathbb{1}.}$$

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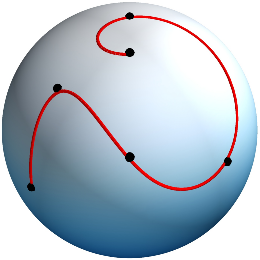
Motivation: Want to guide quantum trajectory through a series of given states at given times. Ideally one would like to do this with a constant Hamiltonian, but this cannot be done in general $\rightsquigarrow$ one looks for Hamiltonian $H(t)$ with **least change**.

Problem statement

Let a set of quantum states $|\phi_1\rangle$, $|\phi_2\rangle$, $\cdots$, $|\phi_m\rangle$ and a set of times t_1, t_2, $\cdots$, t_m be given. Starting from an initial state $|\psi_0\rangle$ at time $t_0 = 0$, find a time-dependent Hamiltonian $H(t)$ such that the evolution path $|\psi_t\rangle$ passes arbitrarily close to $|\phi_j\rangle$ at time $t = t_j$ for all $j = 1, \ldots, m$, and such that the change in the Hamiltonian (in a sense defined later), is minimised.



- The mathematical formulation involves a **cost functional** made up of two terms: One part measures the change in the Hamiltonian along the trajectory. The other one measures the amount of 'mismatch' between trajectory and target states.
- For this purpose, introduce an inner product on $\mathfrak{su}(n+1)$,

$$\boxed{\langle A, B\rangle = -2\,\mathrm{tr}(AB)}$$

and the standard geodesic distance on $\mathbb{CP}^n$,

$$\boxed{D(\psi, \phi) = 2 \arccos \sqrt{\frac{\langle\psi|\phi\rangle\langle\phi|\psi\rangle}{\langle\psi|\psi\rangle\langle\phi|\phi\rangle}}}$$

Link

Cost functional

Given the set of target states $|\phi_1\rangle, \cdots, |\phi_m\rangle$ and times $t_1, \cdots, t_m$, as well as an initial state $|\psi_0\rangle$ and an initial Hamiltonian $H(0) = H_0$, find the minimiser of the **cost functional**

$$\mathcal{J}[U, M, H] = \int_{t_0}^{t_m} \left(\frac{1}{2}\langle \mathrm{i}\dot{H}, \mathrm{i}\dot{H}\rangle + \langle M, \dot{U}U^{-1} + \mathrm{i}H\rangle \right) \mathrm{d}t + \frac{1}{2\sigma^2} \sum_{j=1}^{m} D^2(\underbrace{U(t_j)\psi_0}_{=|\psi_{t_j}\rangle}, \phi_j) \,,$$

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- The minimisation is over curves $U(t) \in SU(n+1)$ and $\mathrm{i}H(t)$, $M(t) \in \mathfrak{su}(n+1)$.
- **Tolerance parameter** σ used to trade off amount of change vs. quality of matching.
- Require **smoothness** of U, H, M on open intervals (t_j, t_{j+1}); and the **continuity** of $U(t)$ and $H(t)$ is assumed everywhere $\rightsquigarrow$ allow for discontinuities of $\dot{H}$ and M at node times t_j.

Euler–Lagrange equations

- On **open intervals** (t_j, t_{j+1}):

$$\boxed{\mathrm{i}\ddot{H} - M = 0, \qquad \dot{M} + [M, \dot{U}U^{-1}] = 0, \qquad \dot{U}U^{-1} + \mathrm{i}H = 0.} \tag{1}$$

At the **nodes** $t = t_j$:

$$\boxed{\dot{H}(t_j^+) - \dot{H}(t_j^-) = 0,} \qquad \boxed{M(t_j^+) - M(t_j^-) = \frac{D_j}{\sigma^2} F_j.} \tag{2}$$

At the **terminal point**:

$$\boxed{\dot{H}(t_m) = 0,} \qquad \boxed{M(t_m) + \frac{D_m}{\sigma^2} F_m = 0.} \tag{3}$$

- Here, $D_j = D(\psi_{t_j}, \phi_j)$ and

$$F_j = J^\sharp(\nabla_1 D(\psi_{t_j}, \phi_j)) = \frac{\langle \psi_{t_j} | \phi_j \rangle |\psi_{t_j}\rangle\langle\phi_j| - \langle\phi_j|\psi_{t_j}\rangle|\phi_j\rangle\langle\psi_{t_j}|}{\sin(D_j)\langle\phi_j|\phi_j\rangle\langle\psi_{t_j}|\psi_{t_j}\rangle},$$

where $J : T^*\mathbb{CP}^n \to \mathfrak{su}(n+1)^*$ is the **cotangent lift momentum map** of the action of $SU(n+1)$ on $\mathbb{CP}^n$.

- Equations (1) and (2) can be integrated for initial values $\dot{H}(0)$ and $M(0)$. A local extremum of the cost functional $\mathcal{J}$ satisfies, in addition, equation (3) at final time.

Geometry of solution curves

1. U(t) is a Riemannian cubic spline

On open intervals (t_j, t_{j+1}), $\boxed{\dddot{H} + \mathrm{i}[H, \ddot{H}] = 0.}$

[[Aside: Lie group G with Riemannian metric γ. A **Riemannian cubic** is a critical curve of the action functional

$$\mathcal{J}[g] = \int_A^B \frac{1}{2}\gamma(D_t\dot{g}, D_t\dot{g})\,\mathrm{d}t$$

with respect to variations with fixed initial/final velocities. If γ is bi-invariant, **second-order Euler–Poincaré** reduction gives

$$\dddot{\xi} - [\xi, \ddot{\xi}] = 0, \qquad \dot{g} = T_e R_g(\xi)$$

Compare with

$$\dddot{H} + \mathrm{i}[H, \ddot{H}] = 0, \qquad \dot{U} = -\mathrm{i}HU.$$

(More details in the Minisymposium Wednesday 18th.)]]

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Indeed, bi-invariant metric associated with the inner product on $\mathfrak{su}(n+1)$ (by left or right translation) $\rightsquigarrow U(t)$ is a **Riemannian cubic** on the open intervals.
Twice continuously differentiable on the whole interval $\rightsquigarrow$ **Riemannian cubic spline**.

Geometry of solution curves (cont'd)

2. Horizontality of the momentum M(t)

Let $\mathfrak{su}(n+1)_\psi$ be the **Lie algebra of the stabilizer** of $|\psi\rangle$ and $\mathfrak{su}(n+1)_\psi^\perp$ its orthogonal complement, the **horizontal space** at $|\psi\rangle$.

Lemma: $\boxed{M(t) \in \mathfrak{su}(n+1)^\perp_{\psi_t},}$ where $|\psi_t\rangle = U(t)|\psi_0\rangle$.

Proof.

Strategy: Final time $\rightsquigarrow$ initial time.

Terminal point: $M(t_m) = -\frac{D_m}{\sigma^2} J^\sharp(\nabla_1 D(\psi_{t_m}, \phi_m)) \Rightarrow$ true at final time, since

$$\left\langle J^\sharp(\alpha_\psi), \xi \right\rangle = \langle J(\alpha_\psi), \xi \rangle_{\mathfrak{su}^* \times \mathfrak{su}} = \langle \alpha_\psi, \xi_{\mathbb{CP}^n}(\psi) \rangle_{T^*\mathbb{CP}^n \times T\mathbb{CP}^n} .$$

Open intervals: $\dot{M} + [M, \dot{U}U^{-1}] = 0 \Rightarrow M(t)$ evolves under the Ad-action (conjugation) of $U(t)$. So does the horizontal space $\mathfrak{su}(n+1)_\psi^\perp \Rightarrow$ true on the open interval (t_{m-1}, t_m).

Node times: $M(t_j^-) = M(t_j^+) - \frac{D_j}{\sigma^2} J^\sharp(\nabla_1 D(\psi_{t_j}, \phi_j)) \Rightarrow$ preserved by jumps at the nodes $\Rightarrow$ true at all times. ■

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In particular, $\boxed{M(0) \in \mathfrak{su}(n+1)_{\psi_0}^\perp.}$ Search for the optimal $M(0)$ can be **restricted** to this $2n$-dimensional subspace of the $n(n+2)$-dimensional Lie algebra $\mathfrak{su}(n+1)$.

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NB: Still need to optimize $\dot{H}(0)$ over all of $\mathfrak{su}(n+1)$.

Quantum control of $SU(2)$-coherent states

So far: Systems of spin. Extend to coherent state submanifolds.

- Introduced by Glauber (1963) as special states of the quantum harmonic oscillator. Associated with the **Heisenberg group**. Generalized to arbitrary **Lie groups** by Perelomov and Gilmore (1972).
- Coherent states achieve the lower bound in the **Heisenberg uncertainty principle** $\rightsquigarrow$ most closely "resemble" classical states.

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Construction:

- **Symmetric n-particle Hilbert space** $\mathcal{H}_n = \bigotimes_{Sym}^n \mathbb{C}^2 \cong \mathbb{C}^{n+1}$, projectively $\mathbb{CP}^n$.
- $SU(2)$ acts diagonally (rotations of the system as a whole).
- Let $e_2 := (0,1) \in \mathbb{C}^2$ ("spin down state") and take $\boxed{\otimes^n e_2} \in \mathcal{H}_n$. The submanifold of **coherent states** is the $SU(2)$-orbit ,

$$\{U(\otimes^n e_2) | U \in SU(2)\}$$

- Coincides with the image set of the **Veronese embedding** V,

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$$V : \mathbb{CP}^1 \to \mathbb{CP}^n, \quad z \mapsto \otimes^n z.$$

$\Rightarrow$ The quantum spline problem on the coherent state submanifold is **equivalent** to the problem on $\mathbb{CP}^1$. **Reason: (1)** the Veronese embedding commutes with $SU(2)$-action, and **(2)** the natural metric on the coherent state submanifold is a scalar multiple of the metric on $\mathbb{CP}^1$.

Two-level system (n=1)

- Spin-$\frac{1}{2}$ particle in a magnetic field.
- Hamiltonian can be written as $H(t) = \omega(t)\mathbf{n}(t) \cdot \boldsymbol{\sigma} = \sum_{i=1}^{3} \omega(t) n_i(t) \sigma_i$
  $\longrightarrow \omega(t)$ strength of the magnetic field
  $\longrightarrow \mathbf{n}(t)$ direction of the magnetic field
- $\mathbb{CP}^1$ diffeomorphic to the **Bloch sphere** S^2.

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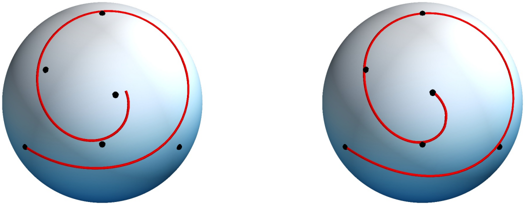
$\rightsquigarrow$ this system can be visualized.

Two-level system (cont'd)

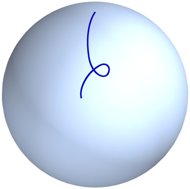
Optimal curve $|\psi_t\rangle$ on state space:



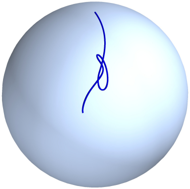
(a) $|\psi_t\rangle$ for $\sigma = 0.04$ (b) $|\psi_t\rangle$ for $\sigma = 0.01$

Two-level system (cont'd)

Optimal Hamiltonian $H(t) = \omega(t)\mathbf{n}(t) \cdot \boldsymbol{\sigma}$ **:**



(c) $\mathbf{n}(t)$ for $\sigma = 0.04$



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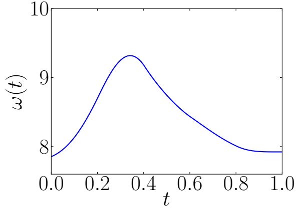
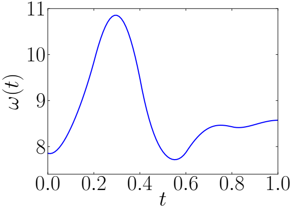


(e) $\omega(t)$ for $\sigma = 0.04$



(f) $\omega(t)$ for $\sigma = 0.01$

Return

Implementation

Optimization via **variational integrator** and **shooting method**. Idea: Pull back the optimization problem to the space of initial conditions $\dot{H}(0)$ and $M(0)$.

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- Integrator is momentum preserving $\Rightarrow M(t) \in \mathfrak{su}(n+1)^{\perp}_{\psi_t}$ satisfied **exactly** on discrete time domain $\Rightarrow$ can restrict search for optimal $M(0)$.
- **Adjoint equations** can be computed $\Rightarrow$ obtain **exact** gradient in an **efficient** way. Becomes important for systems with $n > 1$.

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Optimization via **variational integrator** and **shooting method**. Idea: Pull back the optimization problem to the space of initial conditions $\dot{H}(0)$ and $M(0)$.

Advantages of using variational integrator:

- Conditions at final time: $\dot{H}(t_m) = 0$ and $M(t_m) + D_m F_m / \sigma^2 = 0$.
  Exact discrete version $\Rightarrow$ precise test of convergence to local minimum.
- Integrator is momentum preserving $\Rightarrow$ $M(t) \in \mathfrak{su}(n+1)^{\perp}_{\psi_t}$ satisfied **exactly** on discrete time domain $\Rightarrow$ can restrict search for optimal $M(0)$.
- **Adjoint equations** can be computed $\Rightarrow$ obtain **exact** gradient in an **efficient** way. Becomes important for systems with $n > 1$.
- **Stability** with respect to step-size.

Thank you