A Geometric Perspective on Variational Methods in Quantum Mechanics

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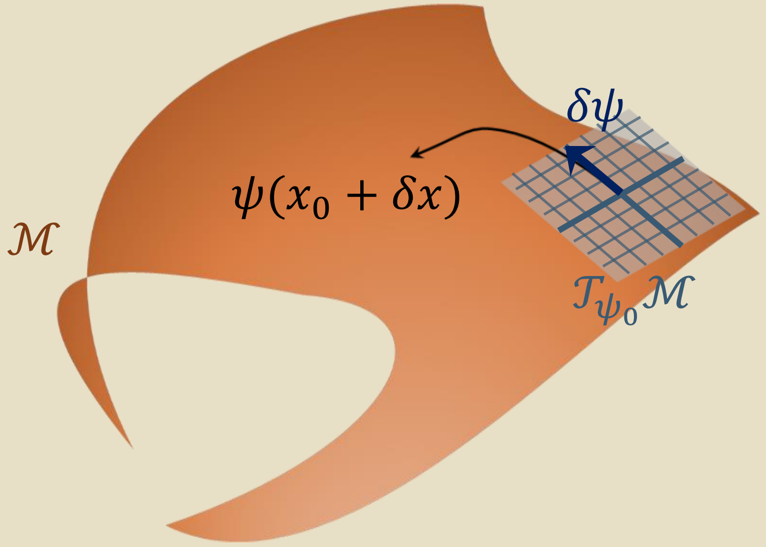


Differential Geometry of Variational Manifolds:

Variational ansatz: real differentiable manifold embedded in Hilbert space

$$\mathcal{M} = \{|\psi(x)\rangle \in \mathcal{H} : x \in A \subseteq \mathbb{R}^n\}$$

Tangent space: local directions of state change under variations of parameters

$$\mathcal{T}_{\psi_0}\mathcal{M} = span_{\mathbb{R}}\left\{|V_\mu(x_0)\rangle = \frac{\partial}{\partial x^\mu}|\psi(x)\rangle\Big|_{x=x_0}\right\}$$

Differential geometry structures: defined on $\mathcal{T}_{\psi_0}\mathcal{M}$ by Hilbert space inner product

$$\langle V_\mu|V_\nu\rangle = \frac{1}{2}(g_{\mu\nu} + i\omega_{\mu\nu})$$

$g_{\mu\nu}$ → Riemannian Metric

$\omega_{\mu\nu}$ → Symplectic Form

Kähler Structures of Variational Manifolds:

- Variational manifolds are:
  - Riemannian manifolds — $g_{\mu\nu}$ - symmetric, definite positive $\longrightarrow$ $G_{\mu\nu} = (g^{-1})^{\mu\nu}$
  - Symplectic manifolds — $\omega_{\mu\nu}$ - anti-symmetric $\longrightarrow$ $\Omega_{\mu\nu} = (\omega^{-1})^{\mu\nu}$

- At each point a **tangent space projector** is defined, thanks to the notion of distance given by the metric

$$\mathbb{P}_{\psi_0}|\psi\rangle \equiv \underset{\phi \in \mathcal{T}_{\psi_0}\mathcal{M}}{\arg\min} \|\phi - \psi\| = |V_\mu\rangle \, \mathrm{G}^{\mu\nu} \, 2 \,\mathrm{Re}\, \langle V_\nu|\psi\rangle$$

- The manifold is a **Kähler manifold** if metric and symplectic structures satisfy the compatibility condition:

$$\begin{array}{c} J = -G\omega \\ J^2 = -\mathbb{I} \end{array} \quad \Longleftrightarrow \quad \begin{array}{c} |X\rangle \in \mathcal{T}_\psi\mathcal{M} \\ \Rightarrow i|X\rangle \in \mathcal{T}_\psi\mathcal{M} \end{array}$$

$\longrightarrow$ *i.e.* the tangent space is a complex linear space

For a Kähler manifold the tangent space projector commutes with multiplication by the imaginary unit

$$\mathbb{P}i|X\rangle = i\mathbb{P}|X\rangle$$

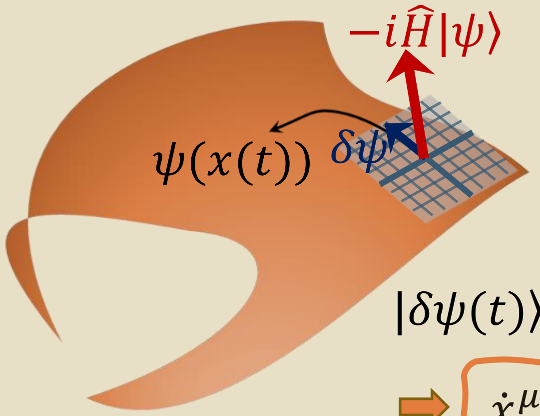
$\longrightarrow$ Important for the equivalence of variational principles

Time Dependent Variational Principle for Real Time Evolution

Aim: define a time evolution on the variational manifold that suitably approximates the Hilbert space evolution generated by the many-body Hamiltonian $\hat{\mathrm{H}}$.

Approaches: two different approaches are possible, corresponding to the two geometric structures of the manifold.

McLachlan Variational Principle



Time evolution defined by applying the *tangent space projector* to exact time evolution:

$$|\delta\psi(t)\rangle = \mathbb{P}_{\psi(t)}(-i\hat{H})|\psi(t)\rangle$$

$$\Rightarrow \quad \dot{x}^{\mu} = -\mathrm{G}^{\mu\nu}\, 2\,\mathrm{Im}\,\langle V_{\nu}|\hat{H}|\psi(t)\rangle$$

Evolution minimises local truncation error:

$$|\delta\psi(t)\rangle = \underset{\delta\psi\,\in\,\mathcal{T}_{\psi}\mathcal{M}}{\arg\min}\,\left\|\delta\psi - (-i\hat{H})|\psi(t)\rangle\right\|$$

Dirac Variational Principle

Time evolution defined through *Hamilton equations* on symplectic manifold:

Analogous to classical phase space $\frac{d}{dt}\begin{pmatrix}\vec{q}\\ \vec{p}\end{pmatrix} = \Omega\begin{pmatrix}\partial_q E\\ \partial_p E\end{pmatrix}$

$$\dot{x}^{\mu} = -\Omega^{\mu\nu}\,\partial_{\nu}E(x)$$

with $E(x) = \langle\psi(x)|\hat{H}\,|\psi(x)\rangle$

Evolution minimises Schrödinger action:

$$\int \mathcal{L}(x,\dot{x})\,dt = \int \mathrm{Re}\langle\psi(x)|\,(i\frac{d}{dt} - \hat{H})\,|\psi(x)\rangle\,dt$$

Properties of Real Time Evolutions

McLachlan Variational Principle

If, for an observable $\hat{A}$,

- $\hat{A}|\psi\rangle \in \mathcal{T}_{\psi}\mathcal{M}, \ \forall \psi \in \mathcal{M}$
- $[\hat{H}, \hat{A}] = 0$

then $A(t) \equiv \langle \psi(t)|\hat{A}|\psi(t)\rangle$ is a constant of motion.

Dirac Variational Principle

- The energy $E(x) = \langle \psi(x)|\hat{H}\,|\psi(x)\rangle$ is always conserved.
- A state that minimises the energy on the variational manifold (approximate ground state) is a stationary point of time evolution.

Kähler equivalence

The Dirac and McLachlan variational principles are equivalent for every Hamiltonian
iff
the variational manifold is Kähler

Indeed the corresponding equations of motion can be written as

$\mathbb{P}_{\psi}\,(\frac{d}{dt} + i\,\hat{H}\,)|\psi\rangle = 0$ *McLachlan*

$\mathbb{P}_{\psi}\,(i\frac{d}{dt} - \,\hat{H}\,)|\psi\rangle = 0$ *Dirac*

⇨ Differ by a factor i that, in Kähler manifolds can be commuted through the projector

Geometric insight on linearised time evolution also gives effective approaches for:

- Low-lying **excitation spectrum**
- **Spectral response** functions

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