Ensembles of particles, observables, Lie algebras: Lessons from hybrid quantum-classical systems

Marcel Reginatto

Physikalisch-Technische Bundesanstalt
Braunschweig, Germany

Assumptions of Physics Workshop: Nonadditive Measures and Generalized Probability in Physics

University of Michigan, July 7-8, 2026

Outline

Quantum-classical interactions

What is a hybrid (mixed classical-quantum) system?

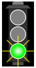
Classical
mechanics

Quantum
mechanics

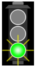

Hybrid system(s)
Which one should you choose? The Opinicus, the Gryphon?

Some motivation

Practical applications: sometimes it is convenient for physical or computational reasons to model some part of a physical system classically.



"Work-in-progress": for some systems, e.g., gravity, there is no full quantum theory yet.



- What happens if gravity is treated classically and matter is described by quantum fields?
- Models where classical gravity (GR) interacts with quantum matter (QFT) may be useful for QG.

Foundations of physics: there is the hope that the study of hybrid systems can give us insight into problems in the foundations of physics.

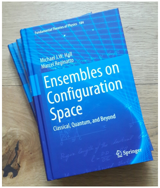
Finding a physically consistent approach is highly nontrivial!

- Classical mechanics and quantum mechanics are formulated using very different mathematical structures.
  $\rightarrow$ it is necessary to find a "common ground."

- Conceptual issues, i.e., uncertainty principle, superposition, etc.
  $\rightarrow$ what parts of classical, quantum mechanics are preserved when describing a mixed system?
  And How?

- $\Rightarrow$ Many, many "*variations on a theme*."

Ensembles on configuration space: classical, quantum and hybrid



Michael J. W. Hall and Marcel Reginatto, *Ensembles on Configurations Space: Classical, Quantum, and Beyond* (Springer)

Ensembles on configuration space: a Hamiltonian approach

Basic idea: Describe ensembles of physical systems by:

- a probability density $P(q)$ on configuration space,
- a canonically conjugate quantity $S(q)$,
- an *ensemble Hamiltonian* $\mathcal{H}[P, S]$.

The *state* of a system is described by $P(q)$ and $S(q)$.

The *equations of motion* for P and S are

$$\frac{\partial P}{\partial t} = \{P, \mathcal{H}\} = \frac{\delta \mathcal{H}}{\delta S}, \qquad \frac{\partial S}{\partial t} = \{S, \mathcal{H}\} = -\frac{\delta \mathcal{H}}{\delta P}.$$

No physics yet! Just dynamics of probabilities.

Example: non-relativistic particles in CM

Ensemble Hamiltonian for two *classical* particles:

$$\mathcal{H}_{CC}[P,S] = \int d^3q_1\, d^3q_2\; P\left[\frac{|\nabla_1 S|^2}{2M_1} + \frac{|\nabla_2 S|^2}{2M_2} + V(\mathbf{q}_1,\mathbf{q}_2)\right].$$

Equations of motion:

$$\begin{aligned}
\frac{\partial S}{\partial t} &+ \frac{|\nabla_1 S|^2}{2M_1} + \frac{|\nabla_2 S|^2}{2M_2} + V(\mathbf{q}_1,\mathbf{q}_2) = 0,\\
\frac{\partial P}{\partial t} &+ \nabla_1\cdot\left(P\frac{\nabla_1 S}{M_1}\right) + \nabla_2\cdot\left(P\frac{\nabla_2 S}{M_2}\right) = 0.
\end{aligned}$$

The equations are

- *Hamilton-Jacobi equation*
- *Continuity equation*

Example: non-relativistic particles in QM

Ensemble Hamiltonian for two *quantum* particles:

$$\mathcal{H}_{QQ}[P,S] = \mathcal{H}_{CC}[P,S] + \frac{\hbar^2}{4}\int d^3x_1\, d^3x_2\; P\left(\frac{|\nabla_1 P|^2}{2m_1\; P^2} + \frac{|\nabla_2 P|^2}{2m_2\; P^2}\right).$$

Equations of motion:

$$\frac{\partial S}{\partial t} + \frac{|\nabla_1 S|^2}{2m_1} + \frac{|\nabla_2 S|^2}{2m_2} + V(\mathbf{x}_1,\mathbf{x}_2) + \frac{\hbar^2}{2}\left(\frac{\nabla_1^2\sqrt{P}}{m_1\sqrt{P}} + \frac{\nabla_2^2\sqrt{P}}{m_2\sqrt{P}}\right) = 0,$$

$$\frac{\partial P}{\partial t} + \nabla_1\cdot\left(P\frac{\nabla_1 S}{m_1}\right) + \nabla_2\cdot\left(P\frac{\nabla_2 S}{m_2}\right) = 0.$$

The *canonical transformation* $\psi := \sqrt{P}\; e^{iS/\hbar}$ leads to

$$i\hbar\frac{\partial\psi}{\partial t} = \frac{-\hbar^2}{2m_1}\nabla_1^2\psi + \frac{-\hbar^2}{2m_2}\nabla_2^2\psi + V(\mathbf{x}_1,\mathbf{x}_2)\,\psi.$$

(See Kibble's "Geometrization of Quantum Mechanics")

Observables

- *Observables* are functionals $A[P, S]$ that satisfy certain requirements.

- For example, the transformation generated by any $A[P, S]$ must preserve $\int d^3q\, P(\mathbf{q}) = 1$. This leads to gauge invariance under $S \rightarrow S + c$,

$$A[P, S + c] = A[P, S].$$

- We will also require that observables be homogeneous of degree one in P; i.e.

$$A[\lambda P, S] = \lambda\, A[P, S] \tag{1}$$

  where $\lambda > 0$ is a constant. Then A can be interpreted as an ensemble average.

Classical and quantum observables - Lie algebras

Observables are functionals $A[P, S]$.

$\rightarrow$ Dual role: as observables *and* generators of canonical.

$\rightarrow$ Closed Lie algebra under the Poisson bracket.

Let $f(\mathbf{q}, \mathbf{p})$ be a classical phase space function.

Define
$C_f[P, S] := \int d^3q\, P\, f(\mathbf{q}, \nabla S)$.

The Poisson bracket for the *classical observables* is isomorphic to the *phase space Poisson bracket,*

$$\{C_f, C_g\} = C_{\{f,g\}}.$$

Let $\hat{M}$ be a quantum operator.

Define
$Q_{\hat{M}}[P, S] := \langle \psi | \hat{M} | \psi \rangle$
$= \int d^3x\, d^3x'\, \sqrt{PP'}\, e^{i(S-S')/\hbar} \langle x' | \hat{M} | x \rangle$.

The Poisson bracket fo ther *quantum observables* is isomorphic to the *commutator on Hilbert space*,

$$\{Q_{\hat{M}}, Q_{\hat{N}}\} = Q_{[\hat{M},\hat{N}]/i\hbar}.$$

Observables, local energy and momentum densities

- Position, momentum observables: $\int d^3q\, P\, \mathbf{q}$, $\int d^3q\, P\nabla S$
- Local energy density: Since $\mathcal{H}[\lambda P, S] = \lambda \mathcal{H}[P, S]$, then

$$\mathcal{H} = \int d^3q\, P \frac{\delta \mathcal{H}}{\delta P} = -\int d^3q\, P \frac{\partial S}{\partial t} = -\langle \partial S / \partial t \rangle.$$

- Local momentum density: $\int d^3q\, P\nabla S$ is the canonical infinitesimal generator of translations,

$$\delta P(\mathbf{q}) = \delta \mathbf{q} \cdot \left\{ P, \int d^3q\, P\nabla S \right\}_{PB} = -\delta \mathbf{q} \cdot \nabla P,$$
$$\delta S(\mathbf{q}) = \delta \mathbf{q} \cdot \left\{ S, \int d^3q\, P\nabla S \right\}_{PB} = -\delta \mathbf{q} \cdot \nabla S.$$

Example: hybrid quantum-classical system

Ensemble Hamiltonian for a *hybrid quantum system* :

$$\begin{aligned}\mathcal{H}_{QC}[P,S] &= \mathcal{H}_Q[P,S] + \mathcal{H}_C[P,S] + \mathcal{H}_{int}[P,S] \\ &= \int d^3x\, d^3q\, P\left(\frac{|\nabla_x S|^2}{2m} + \frac{\hbar^2}{P^2}\frac{|\nabla_x P|^2}{8m} + \frac{|\nabla_q S|^2}{2M} + V\right).\end{aligned}$$

Equations of motion:

$$\begin{aligned}\frac{\partial S}{\partial t} &+ \frac{|\nabla_x S|^2}{2m} + \frac{\hbar^2}{2m}\frac{\nabla_x^2\sqrt{P}}{\sqrt{P}} + \frac{|\nabla_q S|^2}{2M} + V(\mathbf{x},\mathbf{q}) = 0, \\ \frac{\partial P}{\partial t} &+ \nabla_x\cdot\left(P\frac{\nabla_x S}{m}\right) + \nabla_q\cdot\left(P\frac{\nabla_q S}{M}\right) = 0.\end{aligned}$$

Quantum and classical probability densities follow from

$$P_C(\mathbf{q}) := \int d^3x\, P(\mathbf{x},\mathbf{q}), \qquad P_Q(\mathbf{x}) := \int d^3q\, P(\mathbf{x},\mathbf{q}).$$

Hybrid van Hove theory

M. Reginatto, A. D. Bermúdez Manjarres, and S. Ulbricht, *Classical and mixed classical-quantum systems from van Hove's unitary representation of contact transformations*, J. Phys.: Conf. Ser. **3107** (2025) 012037

A preview of things to come: Dirac's proposal for quantization revisited

- Dirac's four basic requirements, or *rules*, for any set of operators $\hat{\mathcal{D}}_F$ representing observables $F(\mathbf{q}, \mathbf{p})$:
  - Linearity rule: $\hat{\mathcal{D}}_{aF+bG} = a\hat{\mathcal{D}}_F + b\hat{\mathcal{D}}_G$
  - Power rule: $\hat{\mathcal{D}}_{F^n} = (\hat{\mathcal{D}}_F)^n$
  - Identity rule: $\hat{\mathcal{D}}_1 = \hat{1}$
  - "Poisson bracket $\rightarrow$ commutator": $[\hat{\mathcal{D}}_F, \hat{\mathcal{D}}_G] = i\hbar\hat{\mathcal{D}}_{\{F,G\}}$

- Dirac's requirements for $\hat{\mathcal{D}}_F$ are *inconsistent*
  - Three out of four are possible

- The Schrödinger operators do not satisfy the 4th rule
  - Groenewold-van Hove theorem

- The van Hove operators do not satisfy the 2nd rule
  - van Hove observables do not form a product algebra

Unitary representation of contact transformations

Léon van Hove, *Sur certaines représentations unitaires d'un groupe infini de transformations*, translated as *On Certain Unitary Representations of an Infinite Group of Transformations* (World Scientific, Singapore, 2001).

- van Hove considers the group Γ of one-to-one, infinitely differentiable point transformation of the space $(s, p_1, ..., p_n, q_1, ..., q_n)$ leaving $(ds - \sum_j p_j dq_j)$ invariant.
- van Hove constructs a representation $\mathcal{R}$ of Γ by unitary transformation in Hilbert space.
- van Hove shows that $\mathcal{R}$ is reducible and that it is the sum of a family of irreducible representations $\mathcal{R}^{(\alpha)}$ that depend on a real parameter α.

van Hove operators

- We consider here the operators corresponding to the particular irreducible representation $\mathcal{R}^{(\alpha)}$ for $\alpha = 1/\hbar$

- Then, given a function $F(\mathbf{q}, \mathbf{p})$ in phase space and its associated Hamiltonian vector field $\xi_F = \{F, \cdot\}$,
  - we introduce the linear function $\theta(F) = F - \mathbf{p} \cdot \nabla_p F$
  - define the van Hove operator

$$\hat{\mathcal{O}}_F = \theta(F) + i\hbar\xi_F = F - \mathbf{p} \cdot \nabla_p F + i\hbar \left(\nabla_q F \cdot \nabla_p - \nabla_p F \cdot \nabla_q \right).$$

- If the Hamiltonian vector field ξ_F is complete, then $\hat{\mathcal{O}}_F$ is essentially self-adjoint.

- States are given by classical wavefunctions $\phi(\mathbf{q}, \mathbf{p}, t)$, with the inner product $\langle \phi | \chi \rangle = \int d^3q d^3p \, \phi^* \chi$.

Isomorphism of Lie algebras

van Hove: the commutator for operators $\hat{\mathcal{O}}_F$ is *isomorphic* to the phase space Poisson bracket, $\left[\hat{\mathcal{O}}_F, \hat{\mathcal{O}}_G\right] = i\hbar\hat{\mathcal{O}}_{\{F,G\}}$.

Sketch of a proof:

$$\hat{\mathcal{O}}_F = F - \mathbf{p}\cdot\nabla_p F + i\hbar\left(\nabla_q F\cdot\nabla_p - \nabla_p F\cdot\nabla_q\right).$$

$$\begin{aligned}
[\hat{\mathcal{O}}_F, \hat{\mathcal{O}}_G]\phi &= i\hbar\left[\{F,(G-\mathbf{p}\cdot\nabla_p G)\} - \{G,(F-\mathbf{p}\cdot\nabla_p F)\}\right]\phi \\
&\quad - \hbar^2\left[\{F,\{G,\phi\}\} - \{G,\{F,\phi\}\}\right] \\
&= i\hbar\left[\{F,(G-\mathbf{p}\cdot\nabla_p G)\} - \{G,(F-\mathbf{p}\cdot\nabla_p F)\}\right]\phi \\
&\quad - \hbar^2\{\{F,G\},\phi\} \\
&= i\hbar\left[\{F,G\} - \mathbf{p}\cdot\nabla_p\{F,G\} + i\hbar\{\{F,G\},\phi\}\right] \\
&= i\hbar\hat{\mathcal{O}}_{\{F,G\}}\phi.
\end{aligned}$$

Interpretation of the classical wavefunction ϕ

$$i\hbar\frac{\partial\phi}{\partial t} = \hat{\mathcal{O}}_H\phi = \left[\left(\frac{\mathbf{p}^2}{2M} - V(\mathbf{x})\right) + i\hbar\left(\nabla_q V\cdot\nabla_p - \frac{\mathbf{p}}{M}\cdot\nabla_q\right)\right]\phi.$$

Write $\phi = \sqrt{\varrho}\, e^{i\sigma/\hbar}$ and evaluate $\bar{\phi}\, i\hbar\,\frac{\partial\phi}{\partial t} = \bar{\phi}\,\hat{\mathcal{O}}_H\,\phi$, then

$$\frac{\partial\varrho}{\partial t} = \nabla_q V\cdot\nabla_p\varrho - \frac{\mathbf{p}}{M}\cdot\nabla_q\varrho = \{\varrho, H\}\,,$$

$$\varrho\left[\frac{\partial\sigma}{\partial t}\right] = \varrho\left[\frac{\mathbf{p}^2}{2M} - V + \nabla_q V\cdot\nabla_p\sigma - \frac{\mathbf{p}}{M}\cdot\nabla_q\sigma\right] = \varrho\left[\mathcal{L} - \{\sigma, H\}\right].$$

$\frac{\partial\varrho}{\partial t} = -\{\varrho, H\} \quad \Rightarrow$ ϱ satisfies the Liouville equation.

$\varrho\left[\frac{\partial\sigma}{\partial t}\right] = \varrho\left[\mathcal{L} - \{\sigma, H\}\right] \Rightarrow$ identify σ with the classical action.

The phase σ is not uniquely determined

Suppose that $\sigma(q, p, t)$ satisfies the equation

$$\frac{\partial \sigma}{\partial t} = \mathcal{L} - \{\sigma, H\}$$

Then

$$\sigma'(q, p, t) = \sigma(q, p, t) + F(H(q, p), \tau(q, p) - t)$$

is also a solution, for arbitrary F and $\{\tau, H\} = 1$.

Expectation values of the operators $\hat{\mathcal{O}}_F$

The expectation value of $\hat{\mathcal{O}}_F$ is given by

$$\begin{aligned}\langle\phi|\hat{\mathcal{O}}_F|\phi\rangle &= \int d\omega\,\varrho\,[(F-\mathbf{p}\cdot\nabla_p F) - (\nabla_q F\cdot\nabla_p\sigma - \nabla_p F\cdot\nabla_q\sigma)] \\ &= \int d\omega\,\varrho\,F + \int d\omega\,\varrho\,[\nabla_p F\cdot(\nabla_q\sigma - \mathbf{p}) - \nabla_q F\cdot\nabla_p\sigma]\end{aligned}$$

Note that the last term on the right hand side vanishes when

$$\varrho\,(\nabla_q\sigma - \mathbf{p}) = 0, \qquad \varrho\nabla_p\sigma = 0$$

We can always choose the phase of the wavefunction so that these conditions are satisfied.

Fixing the phase of the classical wave function

Introduce functions

- $\eta(\mathbf{q},\mathbf{p})$ that satisfies $\{\eta, H\} = \frac{|\mathbf{p}|^2}{2m} - V$,
- $\tau(\mathbf{q},\mathbf{p})$ that satisfies $\{\tau, H\} = 1$.

Set $\sigma = \eta + H(\tau - \tau_0 - t)$ and evaluate the equation for σ,

$$\varrho \left[\frac{\partial\sigma}{\partial t} - \frac{|\mathbf{p}|^2}{2m} + V + \{\sigma, H\}\right] = \varrho \left[\nabla_q\sigma \cdot \frac{\mathbf{p}}{m} - \nabla_p\sigma \cdot \nabla_q V - \frac{|\mathbf{p}|^2}{m}\right] = 0.$$

Consider the case where ϱ is a delta function.

We have motion on a single trajectory, $\dot{\mathbf{q}} = \frac{\mathbf{p}}{M}$, $\dot{\mathbf{p}} = -\nabla_q V$.

$$\Rightarrow \varrho \left[(\nabla_q\sigma - \mathbf{p}) \cdot \dot{\mathbf{q}} + \nabla_p\sigma \cdot \dot{\mathbf{p}}\right] = 0,$$

$$\Rightarrow \varrho \left(\nabla_q\sigma - \mathbf{p}\right) = \nabla_p\sigma = 0.$$

Absence of a superposition principle

- If we were to define a classical wavefunction via a linear superposition, $\phi = \phi_1 + \phi_2$, the density ϱ and phase of ϕ would be given by

$$\begin{aligned} \varrho &= \varrho_1 + \varrho_2 + 2\sqrt{\varrho_1 \varrho_2}\, \cos[(\sigma_1 - \sigma_2)/\hbar], \\ \sigma &= \hbar \tan^{-1}\left(\frac{\sqrt{\varrho_1}\sin(\sigma_1/\hbar) + \sqrt{\varrho_2}\sin(\sigma_2/\hbar)}{\sqrt{\varrho_1}\cos(\sigma_1/\hbar) + \sqrt{\varrho_2}\cos(\sigma_2/\hbar)} \right). \end{aligned}$$

- A superposition does not lead to another classically acceptable wave function.

- *No superposition principle and interference*.

- *Classical mixtures* are perfectly fine!
  - $\Omega(q, p, q', p') = \Sigma_\alpha a_\alpha \phi^*_\alpha(q, p)\phi_\alpha(q', p')$

Absence of an uncertainty principle (I)

The commutator of the generators/observables representing p and p is

$$
\begin{aligned}
[\hat{\mathcal{O}}_q, \hat{\mathcal{O}}_p] &= \left(q + i\hbar\frac{\partial}{\partial p}\right)\left(-i\hbar\frac{\partial}{\partial q}\right) - \left(-i\hbar\frac{\partial}{\partial q}\right)\left(q + i\hbar\frac{\partial}{\partial p}\right) \\
&= i\hbar
\end{aligned}
$$

Consider the ket $|\alpha\rangle = (\hat{\mathcal{O}}_q + i\lambda\hat{\mathcal{O}}_p)|\phi\rangle$ and assume for simplicity that $\langle\phi|\hat{\mathcal{O}}_q|\phi\rangle = \langle\phi|\hat{\mathcal{O}}_p|\phi\rangle = 0$.

$$
\langle\alpha|\alpha\rangle = \langle\phi|\hat{\mathcal{O}}_q\hat{\mathcal{O}}_q|\phi\rangle - \lambda\hbar + \lambda^2\langle\phi|\hat{\mathcal{O}}_p\hat{\mathcal{O}}_p|\phi\rangle \geq 0.
$$

As the last expression is quadratic in λ, the condition that it be non-negative leads to
$\langle\phi|\hat{\mathcal{O}}_q\hat{\mathcal{O}}_q|\phi\rangle\langle\phi|\hat{\mathcal{O}}_p\hat{\mathcal{O}}_p|\phi\rangle \geq \left(\frac{\hbar}{2}\right)^2$.

Absence of an uncertainty principle (II)

A *crucial difference* between the operators $\hat{Q}$, $\hat{P}$ of quantum mechanics and the van Hove operators $\hat{\mathcal{O}}_q$, $\hat{\mathcal{O}}_p$ is that

$$\hat{Q}\hat{Q} = \hat{Q}^2, \qquad \hat{P}\hat{P} = \hat{P}^2,$$
$$\hat{\mathcal{O}}_q\hat{\mathcal{O}}_q \neq \hat{\mathcal{O}}_{q^2}, \qquad \hat{\mathcal{O}}_p\hat{\mathcal{O}}_p \neq \hat{\mathcal{O}}_{p^2}.$$

As a matter of fact,

$$\hat{\mathcal{O}}_q\hat{\mathcal{O}}_q = \left(q + i\hbar\frac{\partial}{\partial p}\right)^2 = q^2 + 2i\hbar q\frac{\partial}{\partial p} - \hbar^2\frac{\partial^2}{\partial p^2},$$
$$\hat{\mathcal{O}}_p\hat{\mathcal{O}}_p = \left(-i\hbar\frac{\partial}{\partial q}\right)^2 = -\hbar^2\frac{\partial^2}{\partial q^2}.$$

Thus $\hat{\mathcal{O}}_q\hat{\mathcal{O}}_q$ and $\hat{\mathcal{O}}_p\hat{\mathcal{O}}_p$ are not even van Hove operators and they are not associated with *any* classical observables.

Classical mechanics à la van Hove: basic equations

- Action of operators.
  $\hat{\mathcal{O}}_F \phi = \left[(F - \mathbf{p} \cdot \nabla_p F) + i\hbar \left(\nabla_q F \cdot \nabla_p - \nabla_p F \cdot \nabla_q \right) \right] \phi.$
- Commutators of operators are isomorphic the Poisson brackets of functions on phase space.
  $\left[\hat{\mathcal{O}}_A, \hat{\mathcal{O}}_B \right] = i\hbar \hat{\mathcal{O}}_{\{A,B\}}.$
- Hamiltonian operator.
  $i\hbar \frac{\partial \phi}{\partial t} = \left[\left(\frac{\mathbf{p}^2}{2M} - V(\mathbf{x}) \right) + i\hbar \left(\nabla_q V \cdot \nabla_p - \frac{\mathbf{p}}{M} \cdot \nabla_q \right) \right] \phi.$
  - $\Rightarrow \quad \frac{\partial \varrho}{\partial t} = -\{\varrho, H\}, \quad \frac{\partial \sigma}{\partial t} = \mathcal{L} - \{\sigma, H\}.$
- Phase of the wavefunction.
  $\sigma = \eta + H(\tau - \tau_0 - t) \quad \Rightarrow \quad \langle \phi | \hat{\mathcal{O}}_F | \phi \rangle = \int d\omega \, \varrho \, F.$

Hybrid system of two interacting particles

- Take a classical particle with phase space coordinates (q, p), add a quantum particle with configuration space coordinate x.
- Classical observables are represented by van Hove operators $\hat{\mathcal{O}}_F$, quantum observables by Schrödinger operators $\hat{F}$.
- The commutator of a classical and quantum observable satisfy $[\hat{\mathcal{O}}_F, \hat{G}] = 0$
- One may define hybrid interaction terms of the form $\hat{\Theta}_I = \sum_k \hat{\mathcal{O}}_{A_k} \hat{B}_k$.
- Equations of motion via a Hybrid Hamiltonian operator

Hybrid system of two non-relativistic particles (I)

Classical particle with phase space coordinates **q**, **p**, add a quantum particle with configuration space coordinates **x**.

The Hamiltonian operator acting on a wavefunction $\psi(\mathbf{q}, \mathbf{p}, \mathbf{x})$ for a hybrid system of two particles interacting via a potential is given by

$$i\hbar \frac{\partial \psi}{\partial t} = \left[\frac{\mathbf{p}^2}{2M} + i\hbar \left(\nabla_q V \cdot \nabla_q - \frac{\mathbf{p}}{M} \cdot \nabla_p \right) \right. \\ \left. - \frac{\hbar^2}{2m} \nabla_x^2 + V(\mathbf{q}, \mathbf{x}) \right] \psi.$$

(See also Gay-Balmaz F, Tronci C, Madelung transform and probability densities in hybrid quantum-classical dynamics, *Nonlinearity* (2019) **33** 5383)

Hybrid system of two non-relativistic particles (II)

Write the hybrid wavefunction $\psi(\mathbf{q}, \mathbf{p}, \mathbf{x}) = \sqrt{\varrho}\, e^{i\sigma/\hbar}$ in terms of Madelung variables.

The previous equation is equivalent to the pair of equations

$$\frac{\partial \varrho}{\partial t} + \left[\frac{\nabla_x \cdot (\varrho \nabla_x \sigma)}{m_Q}\right] + \nabla_q \varrho \cdot \frac{\mathbf{p}}{m_c} - \nabla_p \varrho \cdot \nabla_q V = 0,$$

$$\frac{\partial \sigma}{\partial t} + \left[\frac{|\nabla_x \sigma|^2}{2m_Q} - \frac{\hbar^2}{2m_Q} \frac{\nabla_x^2 \sqrt{\varrho}}{\sqrt{\varrho}}\right] + \nabla_q \sigma \cdot \frac{\mathbf{p}}{m} - \nabla_p \sigma \cdot \nabla_q V = \frac{\mathbf{p}^2}{2m} - V.$$

(See also Gay-Balmaz F, Tronci C, Madelung transform and probability densities in hybrid quantum-classical dynamics, *Nonlinearity* (2019) **33** 5383)

Some remarks...

- The description of classical systems using van Hove operators is an alternative to Koopman-von Neumann.
  - It incorporates aspects of classical mechanics in phase space not captured by the KvN formalism.
  - It clarifies the interpretation of the phase of the classical wavefunction.
  - It does not require a distinction between observables and generators, no need for superselection rules.
  - It provides a counter-example to the assumption that classical observables *must* be commuting operators.
- The description of classical systems can be extended to hybrid systems.
  - The distinction between classical and quantum observables is at the level of Lie algebras.

The geometry of ensembles on configuration space

M. Reginatto, *From probabilities to wave functions: A derivation of the geometric formulation of quantum theory from information geometry*, J. Phys.: Conf. Ser. **538** (2014) 012018

Information geometry

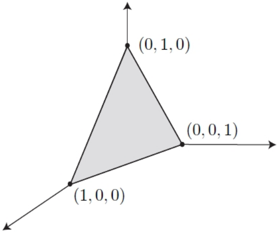
- Classical system, n different states.
- Probabilities P^i which satisfy $P^i \geq 0$, $\sum_i P^i = 1$.
- There is a natural line element given by

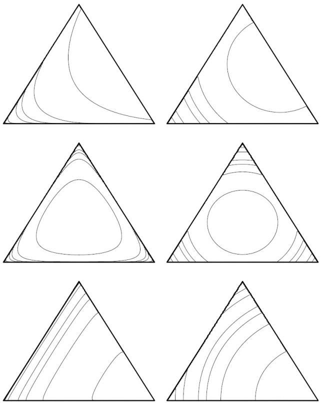
$$ds^2 = G_{ij}\, dP^i\, dP^j = \frac{\alpha}{2P^i}\, \delta_{ij}\, dP^i\, dP^j .$$

- The value of α can not be determined *a priori*; it is usually set to $\frac{1}{2}$. Here, allow α to be a free parameter.
- The metric G_{ij} is known as the **information metric**,

$$G_{ij} = \frac{\alpha}{2P^i}\, \delta_{ij} .$$

Equal distance contours on $\mathbb{P}_2$





Figures: Guy Lebanon, *Riemannian geometry and statistical machine learning*

Uniqueness of the information metric

- N. N. Čencov, based on invariance under "certain probabilistically meaningful transformations" known as *congruent embeddings by a Markov mapping*.
- A simpler proof later provided by L. L. Campbell.
- Markov mappings can be used to map probability spaces of different dimensions; e.g.,

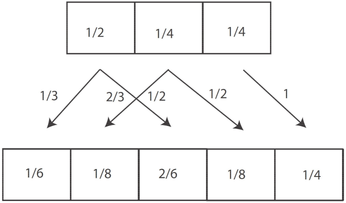


Figure: Guy Lebanon, *Riemannian geometry and statistical machine learning*

Invariance of the information metric under Markov mappings

- Consider the simple example of a Markov mapping given by ($0 < k < 1$):
$$(P^1, P^2) \to (\tilde{P}^1, \tilde{P}^2, \tilde{P}^3) := (P^1, kP^2, (1-k)P^2).$$
- Invariance of the inner product of tangent vectors A, B:

$$\begin{aligned}
< A, B > &= \frac{A^1\, B^1}{P^1} + \frac{A^2\, B^2}{P^2}, \\
< \tilde{A}, \tilde{B} > &= \frac{\tilde{A}^1\, \tilde{B}^1}{\tilde{P}^1} + \frac{\tilde{A}^2\, \tilde{B}^2}{\tilde{P}^2} + \frac{\tilde{A}^3\, \tilde{B}^3}{\tilde{P}^3}, \\
&= \frac{A^1\, B^1}{P^1} + \frac{kA^2\, kB^2}{kP^2} + \frac{(1-k)A^2\, (k-1)B^2}{(1-k)P^2} \\
&= \frac{A^1\, B^1}{P^1} + \frac{A^2\, B^2}{P^2} = < A, B >
\end{aligned}$$

Probabilities in motion: Dynamics and observables

- Introduce additional coordinates S^i canonically conjugate to P^i and a Poisson bracket,

$$\{F, G\} = \sum_i \left(\frac{\partial F}{\partial P^i} \frac{\partial G}{\partial S^i} - \frac{\partial F}{\partial S^i} \frac{\partial G}{\partial P^i} \right).$$

- The equations of motion for P^i and S^i are $\dot{P}^i = \{P^i, H\}$, $\dot{S}^i = \{S^i, H\}$ where H is the Hamiltonian.

- Observables are functions $A(P, S)$.

  The A are not arbitrary! For example, the canonical transformations generated by A must preserve $\sum_i P^i = 1$. This particular condition leads to the *gauge invariance* $S^i \to S^i + \chi$.

Symplectic geometry

- As is well known, the Poisson bracket can be rewritten geometrically as

$$\{F, G\} = (\partial F/\partial P\,,\ \partial F/\partial S)\ \Omega \begin{pmatrix} \partial G/\partial P \\ \partial G/\partial S \end{pmatrix}.$$

- Ω is the corresponding symplectic form, given in this case by

$$\Omega = \begin{pmatrix} 0 & \mathbf{1} \\ -\mathbf{1} & 0 \end{pmatrix},$$

where **1** is the unit matrix in n dimensions.

- We have a symplectic structure and a corresponding *symplectic geometry*.

A more general metric

- Can we extend the metric $G_{ij} = \frac{\alpha}{2P^i}\,\delta_{ij}$, which is only defined on the subspace of probabilities P, to the full space of P *and* S?
- It can be done, but certain conditions which ensure the compatibility of the metric and symplectic structures have to be satisfied.
- These conditions amount to requiring that the space have a Kähler structure.
- *The natural geometry of the space of probabilities in motion is a Kähler geometry*.

Kähler geometry

- A Kähler structure brings together metric, symplectic and complex structures in a harmonious way.

- The Kähler conditions are:

$$\begin{aligned} \Omega_{ab} &= g_{ac} J^c_{\ b} \,, && (2) \\ J^a_{\ c} g_{ab} J^b_{\ d} &= g_{cd} \,, && (3) \\ J^a_{\ b} J^b_{\ c} &= -\delta^a_{\ c} \,. && (4) \end{aligned}$$

- What to these conditions mean?
  (2) There is some tensor $J^a_{\ b}$ which relates Ω_{ab} and g_{ab},
  (3) The metric g_{ab} has to be Hermitian,
  (4) $J^a_{\ b}$ is a complex structure.

General solution of the Kähler conditions

- The metric over the full space will take the form

$$g_{ab} = \begin{pmatrix} \mathbf{G} & \mathbf{E} \\ \mathbf{E}^T & \mathbf{F} \end{pmatrix},$$

where $\mathbf{G} = \mathtt{diag}(\frac{\alpha}{2P^i})$, and $\mathbf{E}$ and $\mathbf{F}$ are $n \times n$ matrices that need to be determined.

- Using the expression for Ω_{ab}, the solution of the Kähler conditions leads to

$$g_{ab} = \begin{pmatrix} \mathbf{G} & \mathbf{A}^T \\ \mathbf{A} & (\mathbf{1} + \mathbf{A}^2)\mathbf{G}^{-1} \end{pmatrix}, \; J^a_{\ b} = \begin{pmatrix} \mathbf{A} & (\mathbf{1} + \mathbf{A}^2)\mathbf{G}^{-1} \\ -\mathbf{G} & -\mathbf{GAG}^{-1} \end{pmatrix},$$

where the $n \times n$ matrix $\mathbf{A}$ satisfies $\mathbf{GAG}^{-1} = \mathbf{A}^T$ but is otherwise arbitrary.

An additional condition that fixes the matrix $\mathbf{A}$

- To fix the matrix $\mathbf{A}$, use the same strategy that leads to the proof of the uniqueness of the information metric.
- Generalize Markov mappings to *canonical transformations*.
- This requires “nonclassical canonical transformations” which map phase spaces of *different* dimensions.
- Invariance under these “*generalized* Markov mappings” forces $\mathbf{A} = A\mathbf{1}$, where A is a constant.
- A further canonical transformation maps the metric to the particular value $\mathbf{A} = 0$.

An example of a “generalized Markov mapping”

- Consider a system with $P = (P^1, P^2)$, with dynamics determined by a Hamiltonian $H(P^1, P^2, S^1, S^2)$.

- A simple example of a Markov mapping is given by $(0 < k < 1)$:

$$(P^1, P^2) \to (\tilde{P}^1, \tilde{P}^2, \tilde{P}^3) = (P^1, kP^2, (1-k)P^2).$$

- To extend it, introduce the *canonical* transformation

$$\begin{aligned}
(\tilde{P}^1,\ \tilde{P}^2,\ \tilde{P}^3) &= (P^1, \quad kP^2 + P^3 \quad , \quad (1-k)P^2 - P^3), \\
(\tilde{S}^1,\ \tilde{S}^2,\ \tilde{S}^3) &= (S^1, \quad S^2 + (1-k)S^3, \quad S^2 - kS^3 \quad).
\end{aligned}$$

- P^3 and S^3 are constants of the motion. Impose the initial conditions (constraints) $P^3 \approx 0$ and $S^3 \approx 0$.

Transformation to complex coordinates

- Consider the case $\mathbf{A} = 0$. The tensors that define the Kähler structure are

$$\Omega_{ab} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}, \; g_{ab} = \begin{pmatrix} \mathbf{G} & 0 \\ 0 & \mathbf{G}^{-1} \end{pmatrix}, \; J^a_{\ b} = \begin{pmatrix} 0 & \mathbf{G}^{-1} \\ -\mathbf{G} & 0 \end{pmatrix}.$$

- Define $\psi^k = \sqrt{P^k} \exp(iS^k/\alpha)$, $\bar{\psi}^k = \sqrt{P^k} \exp(-iS^k/\alpha)$. This leads to the standard form of a *flat Kähler space*,

$$\Omega_{ab} = \begin{pmatrix} 0 & i\alpha\mathbf{1} \\ -i\alpha\mathbf{1} & 0 \end{pmatrix}, \; g_{ab} = \begin{pmatrix} 0 & \alpha\mathbf{1} \\ \alpha\mathbf{1} & 0 \end{pmatrix}, \; J^a_{\ b} = \begin{pmatrix} -i\mathbf{1} & 0 \\ 0 & i\mathbf{1} \end{pmatrix}$$

- The natural coordinates of the space are ψ^i and $\bar{\psi}^i$. If we set $\alpha = \hbar$, these fundamental variables are precisely the *wave functions* of quantum mechanics.

Transformation to complex coordinates when $A \neq 0$

- When $\mathbf{A} \neq 0$, the tensors g_{ab} and J^a_b are defined by

$$g_{ab} = \begin{pmatrix} \mathbf{G} & A\,\mathbf{1} \\ A\,\mathbf{1} & (1+A^2)\mathbf{G}^{-1} \end{pmatrix}, \quad J^a_b = \begin{pmatrix} A\,\mathbf{1} & (1+A^2)\mathbf{G}^{-1} \\ -\mathbf{G} & -A\,\mathbf{1} \end{pmatrix}.$$

- Define $\phi^k = \sqrt{P^k} \exp\left[i \left(\Lambda\, S^k/\alpha - \gamma \ln \sqrt{P^k} \right) \right]$ with $\Lambda = 1/(1+A^2)$ and $\gamma = -A/(1+A^2)$.

- This *modified* Madelung transformation leads to the standard form of a flat Kähler space,

$$\Omega_{ab} = \begin{pmatrix} 0 & i(\alpha/\Lambda)\mathbf{1} \\ -i(\alpha/\Lambda)\mathbf{1} & 0 \end{pmatrix}, \quad g_{ab} = \begin{pmatrix} 0 & (\alpha/\Lambda)\mathbf{1} \\ (\alpha/\Lambda)\mathbf{1} & 0 \end{pmatrix},$$

$$J^a_b = \begin{pmatrix} -i\mathbf{1} & 0 \\ 0 & i\mathbf{1} \end{pmatrix}.$$

Group of linear unitary transformations (I)

- What transformations are allowed? We want to have the following invariants:
  - Normalization: $\sum_i P^i = \sum_i \bar{\psi}^i \psi^i = 1$,
  - Form invariance of the metric: $d\sigma^2 = 2\alpha \sum_i d\bar{\psi}^i d\psi^i$.

- These two conditions leads to the group of rotations on the $2n$-dimensional sphere.

- To get a third and final condition, we consider infinitesimal transformations of $\bar{\psi}^j$ and $\bar{\psi}^j$,

$$\dot{\psi}^j = -i\,\partial H/\partial \bar{\psi}^j, \quad \dot{\bar{\psi}}^j = i\,\partial H/\partial \psi^j.$$

  where H is a generator of rotations. Then,

$$H = E(t) + M_{jk}\bar{\psi}^j \psi^k + N_{jk}\psi^j \psi^k + \bar{N}_{jk}\bar{\psi}^j \bar{\psi}^k$$

  where $E(t)$ is a arbitrary function of time, M is a Hermitian matrix, and N is symmetric matrix.

Group of linear unitary transformations (II)

- H must be invariant under the gauge transformations $S^j \to S^j + \chi$ (or, equivalently, $\psi \to \psi e^{i\chi}$).

- This leads to

$$N_{jk}\psi^j\psi^k e^{2i\chi} + \bar{N}_{jk}\bar{\psi}^j\bar{\psi}^k e^{-2i\chi} = 0$$

and, differentiating with respect to χ, to

$$2i\,[\,N_{jk}\psi^j\psi^k e^{2i\chi} - \bar{N}_{jk}\bar{\psi}^j\bar{\psi}^k e^{-2i\chi}\,] = 0.$$

- Since these identities must hold for all ψ, it follows that $N_{jk} \equiv 0$, i.e., the ensemble Hamiltonian has the Hermitian form $H = E(t) + M_{jk}\bar{\psi}^j\psi^k$.

- The transformations allowed by the theory are precisely the linear unitary transformations.

Hilbert space and Dirac product

- There is a standard construction that associates a complex Hilbert space with any Kähler space.
- Given two complex vectors ϕ^i and φ^i, define the Dirac product by

$$
\begin{aligned}
\langle\phi|\varphi\rangle &= \frac{1}{2}\left\{(\phi,\bar{\phi})\cdot[g+i\Omega]\cdot\begin{pmatrix}\varphi\\ \bar{\varphi}\end{pmatrix}\right\}\\
&= \frac{1}{2}\left\{(\phi,\bar{\phi})\left[\begin{pmatrix}0 & \mathbf{1}\\ \mathbf{1} & 0\end{pmatrix}+i\begin{pmatrix}0 & i\mathbf{1}\\ -i\mathbf{1} & 0\end{pmatrix}\right]\begin{pmatrix}\varphi\\ \bar{\varphi}\end{pmatrix}\right\}\\
&= \sum_i \bar{\phi}^i\varphi^i.
\end{aligned}
$$

- This suggests that the Hilbert space structure of quantum mechanics is perhaps not as fundamental as its geometrical structure.

Statistical distance (Bhattacharyya, Wootters)

- Two points in probability space, P_A and P_B, joined by a curve $P^i(t)$, $0 \leq t \leq 1$.
- Let $X^i = \sqrt{P^i}$. The length l of the curve is

$$l = \int_0^1 dt \sqrt{G_{ij} \frac{dP^i(t)}{dt} \frac{dP^j(t)}{dt}} = \sqrt{2\alpha} \int_0^1 dt \sqrt{\sum_{i=1}^{n} \left[\frac{dX^i(t)}{dt} \right]^2} .$$

- Impose condition $\sum_i P^i(t) = \sum_i [X^i(t)]^2 = 1$. Then

$$\begin{aligned} d(P_A, P_B) &= \sqrt{2\alpha} \cos^{-1} \left(\sum_i X_A^i X_B^i \right) \\ &= \sqrt{2\alpha} \cos^{-1} \left(\sum_i \sqrt{P_A^i} \sqrt{P_B^i} \right) . \end{aligned}$$

- Same as Bhattacharyya and Wootters provided α is set to the standard value of $\frac{1}{2}$.

Statistical distance in the Kähler space

- Consider two points ψ_A and ψ_B joined by a curve $\psi^i(t)$, $0 \leq t \leq 1$. The generalization of the expression for the distance l is

$$l = \int_0^1 dt \sqrt{g_{ij} \frac{d\psi^i(t)}{dt} \frac{d\bar{\psi}^j(t)}{dt}} = \sqrt{2\alpha} \int_0^1 dt \left| \left(\frac{d\psi(t)}{dt}, \frac{d\psi(t)}{dt} \right) \right| .$$

  where $|(\psi, \psi)| = \sqrt{\sum_i \psi^i \bar{\psi}^i}$.

- Impose the condition $\sum_i \psi^i(t)\bar{\psi}^i(t) = 1$. Then

$$d(\psi_A, \psi_B) = \sqrt{2\alpha}\, cos^{-1} \left|(\psi_A, \psi_B)\right| .$$

- Same as Wootters expression for the statistical distance in quantum mechanics, provided α is set to the standard value of $\frac{1}{2}$.

Remarks

- Some features of this reconstruction of discrete quantum mechanics:
  - **Doubling of the dimensionality of the space** (i.e., $\{P^i\} \to \{P^i, S^i\}$) from dynamical considerations.
  - **Complex structure** from consistency between metric and symplectic structures.
  - **Wave functions** as the natural complex coordinates of the Kähler space.
  - **Unitary transformations** as the group of transformations allowed by the theory.
  - **Hilbert space formulation** expressed in terms of geometrical quantites associated with the Kähler space.
  - **Wootters' statistical distance for quantum mechanics** derived in a purely geometrical way.
- The approach is also applicable to continuous systems.

Conclusion

Discrete quantum mechanics stands at the intersection of information geometry, symplectic geometry, and Kähler geometry.

Thank you for your attention