On connections between three different models of hybrid quantum-classical systems

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Quantum-classical interface in closed and open systems
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Outline

Quantum-classical interactions

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

Classical
mechanics

Quantum
mechanics

Hybrid system(s)
Which one do you prefer? The Opinicus or the Gryphon?

Finding a physically consistent approach is highly nontrivial!

- Classical mechanics and quantum mechanics are formulated using very different mathematical structures.
  $\rightarrow$ we need to find a "common ground."
- Conceptual issues, i.e., uncertainty principle, superposition, etc.
  $\rightarrow$ what parts of classical, quantum mechanics do we preserve when we describe a mixed system? And How?
- $\Rightarrow$ Many, many "*variations on a theme*."

Ensembles on configuration space

Ensembles on configuration space: a Hamiltonian approach

Basic idea: Describe ensembles of physical systems by:

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

The *state* of a system is described by $P(\mathbf{x})$ and $S(\mathbf{x})$.

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:

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

- Equations of motion:

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

- The equations are:
  - *Hamilton-Jacobi equation*
  - *Continuity equation*

Example: non-relativistic particles in QM

- Ensemble Hamiltonian for two *quantum* particles:

$$\mathcal{H}_{QQ}[P,S] = \mathcal{H}_{CC}[P,S] + \frac{\hbar^2}{4}\int d\mathbf{q}_1\, d\mathbf{q}_2\; P\left(\frac{|\nabla_1 P|^2}{2m_1\; P^2} + \frac{|\nabla_2 P|^2}{2m_2\; P^2}\right).$$

- Equations of motion:

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

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

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

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

- See Kibble's "Geometrization of Quantum Mechanics"

  T. W. B. Kibble, Commun. math. Phys. 65, 189-201 (1979)
  M. Reginatto and M. J. W. Hall, AIP Conf. Proc 1443, 96-103 (2011)

Classical and quantum observables

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

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

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

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

Define

$$C_f[P, S] := \langle f \rangle$$
$$= \int dx\, P\, f(\mathbf{x}, \nabla S).$$

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 (i.e., a Hermitian operator in Hilbert space).

Define

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

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

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

Example: hybrid quantum-classical system

- Ensemble Hamiltonian for an interacting *classical / quantum system* :

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

- Equations of motion:

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

- Quantum and classical probability densities:

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

Reduced density operator, phase space density

- Conditional wavefunction, density operator:

$$\psi(\mathbf{q}|\mathbf{x}) := \sqrt{P(\mathbf{q}|\mathbf{x})}\, e^{iS(\mathbf{q},\mathbf{x})/\hbar}, \qquad P(\mathbf{q}|\mathbf{x}) = P(\mathbf{q},\mathbf{x})/P(\mathbf{x})$$

$$\hat{\rho}_{Q|C} := \int d\mathbf{x}\, P(\mathbf{x})\, |\psi_x\rangle\langle\psi_x|, \qquad |\psi_x\rangle := \int d\mathbf{q}\, \psi(\mathbf{q}|\mathbf{x})\, |\mathbf{x}\rangle$$

- Conditional classical phase density:

$$\rho_{C|Q} := \int d\mathbf{q}\, P_Q(\mathbf{q})\, P(\mathbf{x}|\mathbf{q})\, \delta(\mathbf{p} - \nabla_x S) = \int d\mathbf{q}\, P(\mathbf{q},\mathbf{x})\, \delta(\mathbf{p} - \nabla_x S)$$

- A full description for a hybrid ensemble requires both $P(\mathbf{q},\mathbf{x})$ and $S(\mathbf{q},\mathbf{x})$
  - it *cannot* be equivalently described by $\hat{\rho}_{Q|C}$ and $\rho_{C|Q}$.

An extension of the theory: Hybrid systems with quantum matter fields and a classical gravitational field

- How do you get there?
  - Extend the theory from particles to *fields*.
  - *Hamilton-Jacobi formulation* of GR for classical sector.
  - *Functional Schrödinger equation* for quantum sector.
- Some calculations...
  - Classical CGHS black hole + quantum scalar field (QFT on CST, Hawking radiation).
  - Special solutions for simple cosmological model.
  - Entanglement of quantum fields via classical gravity.

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

Marcel Reginatto and Michael J. W. Hall, *Entangling quantum fields via a classical gravitational interaction*, J. Phys.: Conf. Ser. 1275 012039 (2019)

Hybrid quantum-classical equations from Galilean invariance

Ensembles on configuration space: Representation of the Galilean group

- The Galilean group has 10 generators:

  $\mathbf{T}$: space translations,
  H : time translations,
  $\mathbf{L}$: space rotations,
  $\mathbf{G}$: Galilean transformations ("boosts").

- Look for a representation of the Galilean group in terms of observables,

$$
\begin{aligned}
\{H, T_i\} &= 0, & \{H, L_i\} &= 0, & \{H, G_i\} &= -T_i, \\
\{L_i, T_j\} &= \epsilon_{ijk} T_k, & \{L_i, L_j\} &= \epsilon_{ijk} L_k, & \{L_i, G_j\} &= \epsilon_{ijk} G_k, \\
\{T_i, T_j\} &= 0, & \{T_i, G_j\} &= -M\delta_{ij}, & \{G_i, G_j\} &= 0,
\end{aligned}
$$

  where M is the central charge.

Space translations, rotations, and Galilean boosts

- The generators of translations and rotations are the observables

$$\begin{aligned}\mathbf{T}[P,S] &= \int d\mathbf{q}\, d\mathbf{x}\; P\;\left(\nabla_q S + \nabla_x S\right),\\ \mathbf{L}[P,S] &= \int d\mathbf{q}\, d\mathbf{x}\; P\;\left(\mathbf{q}\times\nabla_q S + \mathbf{x}\times\nabla_x S\right).\end{aligned}$$

- The generators of Galilean boost are

$$\mathbf{G}[P,S] = \int d\mathbf{q}\, d\mathbf{x}\; P\;\left(m_Q\mathbf{q} - t\nabla_q S + m_C\mathbf{x} - t\nabla_x S\right),$$

where t is the time.

Time translations and Galilean invariance

- The generator of time translations H is the hybrid ensemble Hamiltonian (energy observable),

$$
\begin{aligned}
H[P,S] &= \mathcal{H}_{QC}[P,S] = \mathcal{H}_{Q}[P,S] + \mathcal{H}_{C}[P,S] + \mathcal{H}_{int}[P,S] \\
&= \int d\mathbf{q}\, d\mathbf{x}\, P \left[\frac{1}{2m_Q} \left(|\nabla_q S|^2 + \frac{\hbar^2}{4P^2} |\nabla_q P|^2 \right) \right. \\
&\qquad \left. + \frac{1}{2m_C} |\nabla_x S|^2 + V(|\mathbf{q} - \mathbf{x}|) \right] .
\end{aligned}
$$

- The term that leads to the quantum potential in the equations of motion follows if you require
  - Galilean invariance
  - No changes to the continuity equation
  - Additivity of the ensemble Hamiltonian for independent, non-interacting subsystems
  - Equations of at most second order in the derivatives of P
- => *Non-classical particles are quantum particles*!

Ensembles on phase space

Ensembles on phase space: A Hamiltonian approach

Basic idea: Describe ensembles of physical systems by:

- a probability density $\varrho(\mathbf{x}, \mathbf{p})$ on phase space,
- a canonically conjugate quantity $\sigma(\mathbf{x}, \mathbf{p})$: the action,
- an ensemble Hamiltonian $\mathcal{H}[\varrho, \sigma]$.

The *equations of motion* for ϱ and σ are

$$\frac{\partial \varrho}{\partial t} = \{\varrho, \mathcal{H}\} = \frac{\delta \mathcal{H}}{\delta \sigma}, \qquad \frac{\partial \sigma}{\partial t} = \{\sigma, \mathcal{H}\} = -\frac{\delta \mathcal{H}}{\delta \varrho}.$$

We now look for an ensemble Hamiltonian that leads to appropriate evolution equations for ϱ and σ.

Example: non-relativistic particle in CM (I)

Classical particle with Hamiltonian and Lagrangian

$$H = \frac{|\mathbf{p}|^2}{2m} + V(\mathbf{x}), \qquad L = \frac{|\mathbf{p}|^2}{2m} - V(\mathbf{x}).$$

- Require that ϱ satisfy the Liouville equation,

$$\frac{\partial \varrho}{\partial t} + \nabla_x \varrho \cdot \frac{\mathbf{p}}{m} - \nabla_p \varrho \cdot \nabla_x V = 0.$$

- Identify σ with the action in phase space, so that

$$\frac{d\sigma}{dt} = \frac{\partial \sigma}{\partial t} + \{\sigma, H\} = L,$$

which implies

$$\frac{\partial \sigma}{\partial t} + \nabla_x \sigma \cdot \frac{\mathbf{p}}{m} - \nabla_p \sigma \cdot \nabla_x V = \frac{\mathbf{p}^2}{2m} - V.$$

Example: non-relativistic particle in CM (II)

The pair of equations

$$\begin{aligned}\frac{\partial \varrho}{\partial t} + \nabla_x \varrho \cdot \frac{\mathbf{p}}{m} - \nabla_p \varrho \cdot \nabla_x V &= 0 \\ \frac{\partial \sigma}{\partial t} + \nabla_x \sigma \cdot \frac{\mathbf{p}}{m} - \nabla_p \sigma \cdot \nabla_x V &= \frac{\mathbf{p}^2}{2m} - V\end{aligned}$$

are equivalent to the Koopman-van Hove equations for a classical wavefunction $\psi(\mathbf{x}, \mathbf{p}) = \sqrt{\varrho}\, e^{i\sigma/\hbar}$.(*)

The corresponding ensemble Hamiltonian is given by

$$\mathcal{H}_C = \int d\mathbf{x} d\mathbf{p}\, \varrho \left[\left(\nabla_x \sigma \cdot \frac{\mathbf{p}}{m} - \frac{\mathbf{p}^2}{2m} \right) + V - \nabla_p \sigma \cdot \nabla_x V \right].$$

* See e.g. Gay-Balmaz, F., Tronci, C., *Madelung transform and probability densities in hybrid quantum-classical dynamics*. Nonlinearity, 33 (2019), n. 10, 5383-5424

The connection between classical ensembles in configuration space and phase space

- The density ϱ is mapped to a *mixture* in configuration space,

$$\rho(\mathbf{x}, \mathbf{p}) = \int d\boldsymbol{\alpha}\ w(\alpha) P(\mathbf{x}|\boldsymbol{\alpha})\ \delta(\mathbf{p} - \nabla_x S(\mathbf{x}; \boldsymbol{\alpha})).$$

- The equations of motion are mapped correctly.
  - To show this you need to use properties of the actions $S(\mathbf{x})$ in configuration space and $\sigma(\mathbf{x}, \mathbf{p})$ in phase space.
- The two ensemble theories are *different*
  - Definitions of observables and of generators of transformations are not the same in both theories.

Ensembles on phase space: Hybrid equations from Galilean invariance

- The Galilean group has 10 generators:
  T : space translations,
  H : time translations,
  L : space rotations,
  G : Galilean transformations ("boosts").

- Look for a representation of the Galilean group in terms of observables,

$$\begin{array}{rclll} \{H, T_i\} & = & 0, & \{H, L_i\} = 0, & \{H, G_i\} = -T_i, \\ \{L_i, T_j\} & = & \epsilon_{ijk} T_k, & \{L_i, L_j\} = \epsilon_{ijk} L_k, & \{L_i, G_j\} = \epsilon_{ijk} G_k, \\ \{T_i, T_j\} & = & 0, & \{T_i, G_j\} = -M\delta_{ij}, & \{G_i, G_j\} = 0, \end{array}$$

  where M is the central charge.

Space translations, rotations, and Galilean boosts

- Generators of translations and rotations,

$$\begin{aligned}
\mathbf{T}[\varrho,\sigma] &= \int d\mathbf{q}\, d\mathbf{x}\, d\mathbf{p}\; \varrho\; \left(\nabla_q\sigma + \nabla_x\sigma\right), \\
\mathbf{L}[\varrho,\sigma] &= \int d\mathbf{q}\, d\mathbf{x}\, d\mathbf{p}\; \varrho\; \left(\mathbf{q}\times\nabla_q\sigma + \mathbf{x}\times\nabla_x\sigma + \mathbf{p}\times\nabla_p\sigma\right).
\end{aligned}$$

- Generators of Galilean boosts,

$$\mathbf{G}[\varrho,\sigma] = \int d\mathbf{q}\, d\mathbf{x}\, d\mathbf{p}\; \varrho\; \left(m_Q\mathbf{q} - t\nabla_q\sigma + m_C\left(\mathbf{x} - \nabla_p\sigma\right) - t\nabla_x\sigma\right),$$

where t is the time.

Time translations and Galilean invariance

- The generator of time translations H is

$$
\begin{aligned}
H[\varrho,\sigma] &= \mathcal{H}_{QC}[\varrho,\sigma] = \mathcal{H}_{Q}[\varrho,\sigma] + \mathcal{H}_{C}[\varrho,\sigma] + \mathcal{H}_{int}[\varrho,\sigma] \\
&= \int d\mathbf{q}\, d\mathbf{x}\, d\mathbf{p}\ \varrho\ \Bigg[\frac{1}{2m_Q}\left(|\nabla_q\sigma|^2 + \frac{\hbar^2}{4\varrho^2}|\nabla_q\varrho|^2\right) \\
&\qquad + \frac{1}{2m_C}\left(2\nabla_q\sigma\cdot\mathbf{p} - \mathbf{p}^2\right) + V(|\mathbf{q}-\mathbf{x}|) \\
&\qquad - \nabla_p\sigma\cdot\nabla_x V(|\mathbf{q}-\mathbf{x}|)\Bigg] .
\end{aligned}
$$

- The last term in H is required to ensure Galilean invariance and conservation of momentum
- The term that leads to the quantum potential in the equations of motion follows from the *same* consistency requirements as in the case of ensembles on configuration space
  - *Non-classical particles are quantum particles*!

Example: hybrid quantum-classical system

- The equations that follow from the hybrid ensemble Hamiltonian are

$$
\begin{aligned}
\frac{\partial \varrho}{\partial t} + \frac{\nabla_q \cdot (\varrho \nabla_q \sigma)}{m_Q} + \nabla_x \varrho \cdot \frac{\mathbf{p}}{m_c} - \nabla_p \varrho \cdot \nabla_x V &= 0, \\
\frac{\partial \sigma}{\partial t} + \frac{|\nabla_q \sigma|^2}{2m_Q} - \frac{\hbar^2}{2m_Q} \frac{\nabla_q^2 \sqrt{\varrho}}{\sqrt{\varrho}} + \nabla_x \sigma \cdot \frac{\mathbf{p}}{m} - \nabla_p \sigma \cdot \nabla_x V &= \frac{\mathbf{p}^2}{2m} - V.
\end{aligned}
$$

- These equations are equivalent to a complex linear equation for a hybrid wavefunction based on a partial quantization of the Koopman-van Hove equation, $\psi(\mathbf{x}, \mathbf{p}) = \sqrt{\varrho}\, e^{i\sigma/\hbar}$.(*)

* See e.g. Gay-Balmaz, F., Tronci, C., *Madelung transform and probability densities in hybrid quantum-classical dynamics*. Nonlinearity, 33 (2019), n. 10, 5383-5424

Relations between classical models

Relations between classical models

- The classical configuration- and phase-space ensemble approaches are *"essentially" equivalent*
- Introduce the classical phase space wavefunction

  $$\tilde{\psi}(\mathbf{q}, \mathbf{p}) = \sqrt{\varrho}\, e^{i\sigma/\hbar}.$$

  Then the equations for the phase space ensemble can be written as a complex linear equation,

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

  the Koopman-van Hove equation.
- Thus one can now introduce a third, *Hilbert space model* based on the Koopman-van Hove equation.
- The three models are *"essentially" equivalent*

Relations between hybrid models

Relations between hybrid models (I)

- The configuration- and phase-space ensemble approaches are *inequivalent for hybrid systems*
  - $\int d\mathbf{q}\, d\mathbf{x}\, d\mathbf{p}\ \varrho \left(\frac{|\nabla_q \varrho|^2}{\varrho^2} \right) \neq \int d\mathbf{q}\, d\mathbf{x}\ P \left(\frac{|\nabla_q P|^2}{P^2} \right)$

    where $P(\mathbf{q}, \mathbf{x}) = \int d^3p\ \varrho(\mathbf{q}, \mathbf{x}, \mathbf{p})$.

- The terms in blue that lead to the quantum potential in the equations of motion are numerically different for the two models.

- The "quantum potential term" behaves differently in each of the two models:
  - For ensembles on configuration space, it depends on $P(\mathbf{q}, \mathbf{x})$; i.e., on the particles' locations only;
  - For ensembles on phase space, it depends on $\varrho(\mathbf{q}, \mathbf{x}, \mathbf{p})$; i.e., also on the *momentum* of the classical particles.

Relations between hybrid models (II)

- Introduce the hybrid wavefunction

$$\tilde{\psi}(\mathbf{q}, \mathbf{p}) = \sqrt{\varrho}\, e^{i\sigma/\hbar}$$

  Then the equations for the phase space ensemble are equivalent to a complex linear equation,

$$i\hbar \frac{\partial \tilde{\psi}}{\partial t} = \left[-\frac{\hbar^2}{2m_Q} \nabla_q^2 + i\hbar \left(\nabla_x V \cdot \nabla_p - \frac{\mathbf{p}}{m_C} \cdot \nabla_x \right) - \frac{\mathbf{p}^2}{2m_C} + V \right] \tilde{\psi},$$

  which is a hybrid extension of the Koopman-van Hove classical model.

- Thus one can again introduce a third model, a *Hilbert space model* which has the same equations as the ones of the hybrid phase space approach – but which is *not* equivalent to the hybrid theory based on ensembles on configuration space.

Summary

Summary

- We looked at three models that describe classical and hybrid systems.
- For classical systems of particles, the fundamental variables and the equations of motion can be shown to be the same.
- The extension to hybrid systems leads to different models.
  - The model based on ensembles on configuration space differs from the other two models.
  - The models based on ensembles on phase space and the Hilbert space model appear to be to a large extent equivalent.
- "Work in progress."
  - States, observables, generators, measurements, ...