On Quantum-Classical Hybrid Canonical Dynamics

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Abstract

Over the decades, desire of a hybrid of quantum and classical dynamics came from many fields spanning from quantum chemistry to cosmology, from foundations to open system theories, also from such special fields like quantum control. Koopman's quantum formalism of classical dynamics or Wigner's classical phase-space formalism of quantum dynamics are two opposite options to create the hybrid formalism. My topics is about a third option, kind of "in the middle". To construct natural coupling between a classical system's canonical formalism and a quantum system's operator formalism, Aleksandrov constructed a hybrid of the Poisson and Dirac brackets, Gerasimenko proposed an equivalent structure. This is remarkable and useful phenomenology but incorrect mathematically. Additional terms to the hybrid bracket can cure the defect, while the reversibility of the resulting hybrid dynamics becomes lost.

Classical, Quantum, Hybrid

Desires of hybrid dynamics

	CLASSICAL subSYSTEM	QUANTUM subSYSTEM
chemistry	nuclei	electrons
cosmology	gravity	matter
foundations	measuring device	measured system
open systems	reservoir	system of interest
control	measured signal	controlled system

Three Main Options for Hybrid Dynamics

CLASSICAL subSYSTEM		QUANTUM subSYSTEM
quantum-like formalism Koopman	extend$\Rightarrow$	
	$\Leftarrow$extend	classical-like formalism Wigner
classical formalism	$\Rightarrow$coupling$\Leftarrow$ Aleksandrov– –Gerasimenko	quantum formalism

Coupling Classical and Quantum Formalisms

	C subSYSTEM		Q subSYSTEM
State:	$\rho(q,p)$		$\hat{\rho}$
Hamilton:	$H(q,p)$		$\hat{H}$
Motion:	$\dot{\rho} = \{H, \rho\}$		$\dot{\hat{\rho}} = -\frac{i}{\hbar}[\hat{H}, \hat{\rho}]$
	Liouville eq.		von Neumann eq.
	Poisson br.		Dirac br.
	C formalism	⇒coupling⇐	Q formalism
State:		$\hat{\rho}(q,p) \equiv \widehat{\rho}$	
Hamilton:		$\hat{H}(q,p) \equiv \widehat{H}$	
Motion:		$\dot{\widehat{\rho}} = -\frac{i}{\hbar}[\widehat{H}, \widehat{\rho}] + \mathrm{Herm}\{\widehat{H}, \widehat{\rho}\}$	
		AG hybrid eq.	
		Aleksandrov br.	

AG Hybrid Dynamics 1981/82

$$\dot{\widehat{\rho}} = -\frac{i}{\hbar}[\widehat{H}, \widehat{\rho}] + \mathrm{Herm}\{\widehat{H}, \widehat{\rho}\}$$

$$\begin{aligned} \dot{\hat{\rho}}(q,p) = & - \frac{i}{\hbar}\left[\hat{H}(q,p), \hat{\rho}(q,p)\right] + \\ & + \mathrm{Herm}\left(\frac{\partial \hat{H}(q,p)}{\partial p}\frac{\partial \hat{\rho}(q,p)}{\partial q} - \frac{\partial \hat{H}(q,p)}{\partial q}\frac{\partial \hat{\rho}(q,p)}{\partial p}\right) \end{aligned}$$

Useful effective dynamics. But inconsistent mathematically.
D.-Gisin-Strunz 2000: 1D classical particle coupled to Pauli-spin:

$$\hat{H}(q,p) = H_{part}(q,p) + \hat{H}_{spin} + \kappa p \hat{\sigma}_3$$

AG hybrid eq. can destruct positivity $0 \leq \hat{\rho}(q,p)$.
So what?

Quantum Dynamics with Two $\hbar$'s, D. 1995

- Quantize the classical subsystem as well, but with $\hbar' \neq \hbar$
- Couple it to the quantum subsystem of interest. Educated Ansatz: generalization of Dirac bracket $-(i/\hbar)[.,.]$ for two $\hbar$'s.
- Nonunitary dynamics, like a quantum master eq. But!
- Incomplete Lindblad 1976 (GKLS 1976, in fact) master eq.
- Complete it! Add the minimum necessary new terms.
- Take $\hbar' \to 0$

Positivity Preserving Hybrid Dynamics, D. 1995

$$\begin{aligned} \hat{H}(q,p) &= \hat{H}_Q &+ H_C(q,p) &+ C(q,p)\hat{Q} \\ \widehat{H} &= \hat{H}_Q &+ H_C &+ C\hat{Q} \end{aligned}$$

$$\dot{\widehat{\rho}} = -\frac{i}{\hbar}[\widehat{H},\widehat{\rho}] + \mathrm{Herm}\{\widehat{H},\widehat{\rho}\} - \frac{\lambda}{4\hbar^2}[\hat{Q},[\hat{Q},\widehat{\rho}]] + \frac{1}{4\lambda}\{C,\{C,\widehat{\rho}\}\}$$

AG dynamics — decoherence — diffusion

Least added noise: (stregth of decoh.) $\times$ (strength of diff.) $=$ const.

Example: 1D classical particle coupled to Pauli-spin:

$$\hat{H}(q,p) = \hat{H}_Q + (p^2/2m) + \kappa p \hat{\sigma}_3$$

$$\begin{aligned} \dot{\hat{\rho}}(q,p) &= -\frac{i}{\hbar}[\hat{H}_Q,\hat{\rho}(q,p)] + \frac{p}{m}\frac{\partial\hat{\rho}(q,p)}{\partial q} + \kappa \mathrm{Herm}\hat{\sigma}_3\hat{\rho}(q,p) \\ &\quad -\frac{\lambda\kappa^2}{4\hbar^2}[\hat{\sigma}_3,[\hat{\sigma}_3,\hat{\rho}(q,p)]] + \frac{\kappa^2}{4\lambda}\frac{\partial^2\hat{\rho}(q,p)}{\partial q^2} \end{aligned}$$

Positivity $0 \leq \hat{\rho}(q,p)$ guaranteed.

What's That, What's It Good or Not so Good for?

$$\widehat{H} = \hat{H}_Q + H_C + C\hat{Q}$$

$$\dot{\widehat{\rho}} = -\frac{i}{\hbar}[\widehat{H}, \widehat{\rho}] + \mathrm{Herm}\{\widehat{H}, \widehat{\rho}\} - \frac{\lambda}{4\hbar^2}[\hat{Q}, [\hat{Q}, \widehat{\rho}]] + \frac{1}{4\lambda}\{C, \{C, \widehat{\rho}\}\}$$

- Special case of generic Hybrid Master Equations, generic unification of Pauli classical & GKLS quantum kinetic (master) equations, D. 2014
- Good, if interacion is written in the form $\sum C_{.}\hat{Q}_{.}$ (electrodynamics, weak gravity, many linearized couplings)
- Not so good if there is no distigushed expansion $\sum C_{.}\hat{Q}_{.}$ of coupling.

Three Main Options for Hybrid Dynamics — Comparisons?

CLASSICAL subSYSTEM		QUANTUM subSYSTEM
quantum-like formalism Koopman	extend$\Rightarrow$	
	$\Leftarrow$extend	classical-like formalism Wigner
classical formalism	$\Rightarrow$coupling$\Leftarrow$ Aleksandrov– –Gerasimenko +decoherence +diffusion =consistency	quantum formalism

Compare the these three! Take the simplest hybrid coupling:

$$\kappa p \times \sigma_3$$

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