5.3

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NOTETAKER CHECKLIST FORM

(Complete one for each talk.)

Name: ORI KATZ Email/Phone: ORI KATZ. OK @ gmail. com

Speaker's Name: Cesare Tronci

Talk Title: Multi-physics models for hybrid Kinetic-fluid & Classical-quantum systems.

Date: 10 / 12 / 18 Time: 2:00 am / (pm) (circle one)

Please summarize the lecture in 5 or fewer sentences: Describing multi-physics models that take into account on interplay of physical phenomena at different scales poses many challenges. Tronci's talk shows how momentum-map techniques in geometric mechanics provide a powerful unifying framework for multi-physics models of kinetic-fluid & classical-quantum coupling.

CHECK LIST

(This is **NOT** optional, we will **not pay** for **incomplete** forms)

- ☐ Introduce yourself to the speaker prior to the talk. Tell them that you will be the note taker, and that you will need to make copies of their notes and materials, if any.
- ☐ Obtain ALL presentation materials from speaker. This can be done before the talk is to begin or after the talk; please make arrangements with the speaker as to when you can do this. You may scan and send materials as a .pdf to yourself using the scanner on the 3rd floor.
  - **Computer Presentations**: Obtain a copy of their presentation
  - **Overhead**: Obtain a copy or use the originals and scan them
  - **Blackboard**: Take blackboard notes in black or blue **PEN**. We will **NOT** accept notes in pencil or in colored ink other than black or blue.
  - **Handouts**: Obtain copies of and scan all handouts
- ☐ For each talk, all materials must be saved in a single .pdf and named according to the naming convention on the "Materials Received" check list. To do this, compile all materials for a specific talk into one stack with this completed sheet on top and insert face up into the tray on the top of the scanner. Proceed to scan and email the file to yourself. Do this for the materials from each talk.
- ☐ When you have emailed all files to yourself, please save and re-name each file according to the naming convention listed below the talk title on the "Materials Received" check list. (*YYYY.MM.DD.TIME.SpeakerLastName*)
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Geometric multiphysics models for hybrid kinetic-fluid and classical-quantum systems

Cesare Tronci

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Collaborators:
A. Brizard (St Michael's), D. Bondar (Tulane), J. Burby (Courant), E. Camporeale (Amsterdam),
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Hamiltonian systems workshop, 8–12 October 2018, MSRI Berkeley CA, USA

Why multiphysics?

- In complex physical systems, various phenomena emerge at **different scales** (in both time and length)

- in many cases, essentially **different physical phenomena are involved at each scale**, thereby requiring a *different physical description*

- Examples:

  - **Liquid crystals**: macroscopic *fluid-like equations* are coupled to the *rotational motion* governing microscopic rod-like molecules

  - **Magnetized plasmas**: often described by coupling *fluid-like eqns* for the plasma bulk to suitable *kinetic theories* for energetic particles

  - **Molecular dynamics**: heavy nuclei essentially obey *classical dynamics*, while electrons require a full *quantum treatment*

Two challenges in multi-physics modeling

- **Kinetic-fluid models** for magnetized plasmas
  - Fluid & kinetic models for plasmas
  - New hybrid plasma models
- Coupled **classical-quantum dynamics**
  - Koopman wavefunctions for classical mechanics
  - Hybrid classical-quantum wave equation

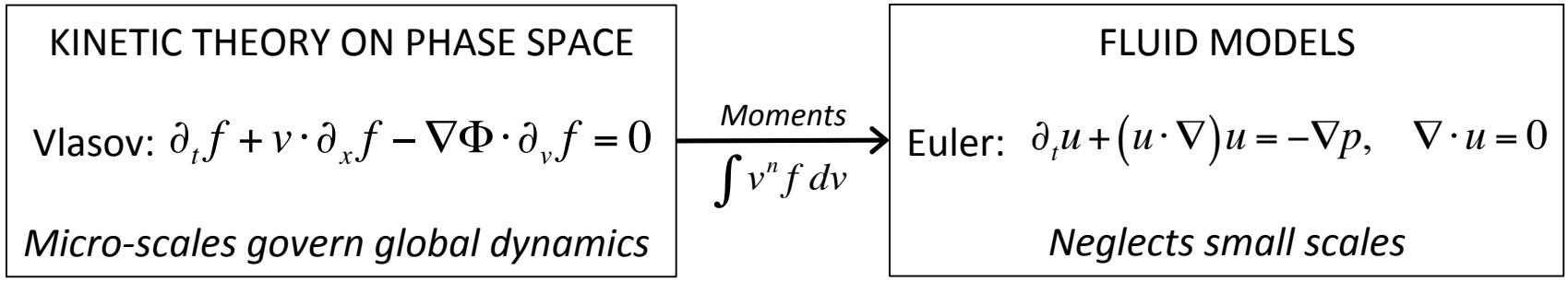
We shall exploit mometum map structures from symplectic geometry!

Geometric hybrid models for magnetized plasmas

Kinetic and fluid models in continuum dynamics

- Fluid models arise from *kinetic equations* by an averaging process

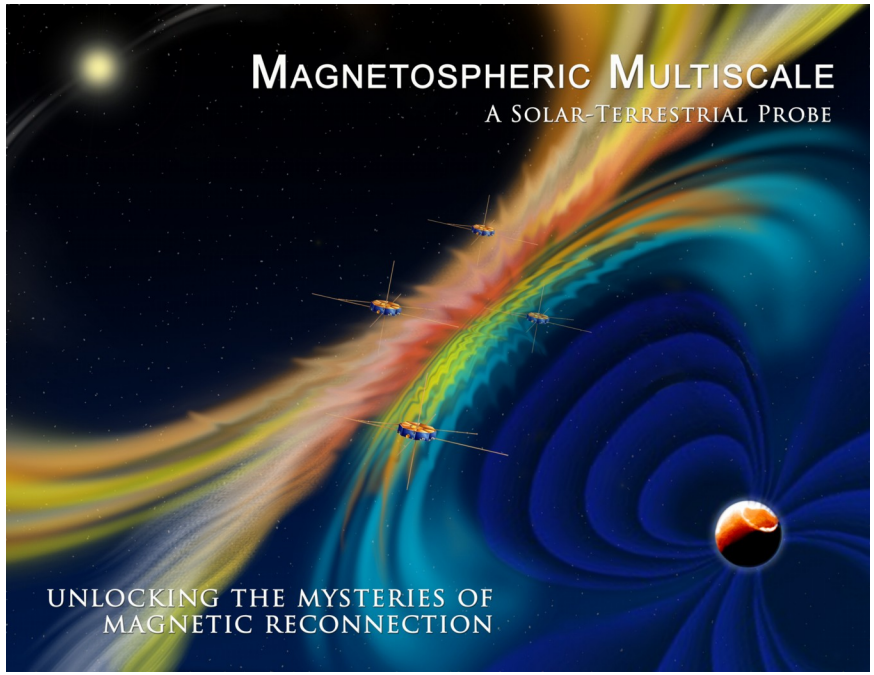
- This averaging process is known in statistics as 'the moment method'



- Fluid closure models generally require low particle energy/temperature

Hybrid kinetic-fluid models for plasma physics

- Plasma simulations are mostly based on fluid (MHD) models
- These are invalidated by the presence of energetic particles
- Then, small-scale processes may control large-scale phenomenology



Energetic Solar wind interacts with Earth's magnetosphere

- *Microscopic effects* need to be considered along with fluid macro-scales
- **Hybrid philosophy: a fluid interacts with a hot particle gas**

Multi-physics approach!

$\rightarrow$ MHD fluid models need to be coupled to kinetic-like equations

- Several coupling options are available, which need special care
- These usually arise by *inserting assumptions in the equations of motion*, cf [Park et al. (1992); Kim et al. (1994); Todo et al. (1995)]

The consistency of hybrid models has been a 20-year open question

. . . *we shall address this problem by using momentum maps!*

Plasma models

- **Particle trajectories** on phase space (Liouville):
  traces particles $(\mathbf{x}(t), \mathbf{p}(t)) \rightarrow$ *solves all details.*

- **Kinetic approach** (Vlasov, Boltzmann):
  probability distribution $f(\mathbf{x}, \mathbf{p}, t) \rightarrow$ *retains most details.*

- **Fluid approach** (MHD, Hall-MHD):
  local averages (momentum $\mathbf{m}(\mathbf{x}, t)$, density $\rho(\mathbf{x}, t)$) $\rightarrow$ *forget details.*

From particle motion to kinetic theory

- Particle simulations for $(\mathbf{x}_s, \mathbf{p}_s)$ solve *all* details, but at huge costs.
- **Kinetic theory**: spread particles across phase-space $\rightarrow$ *probability*
- Averaging processes (BBGKY) lead to the *particle distribution* $f(\mathbf{x}, \mathbf{p})$.
- A *kinetic equation* is an evolution equation for $f(\mathbf{x}, \mathbf{p})$.
- *Collisional* $\rightarrow$ *Boltzmann* (H-theorem)
- *Collisionless* $\rightarrow$ **Vlasov** (mean field model)

$$\partial_t f + \{f, H\} = 0$$

Kinetic approaches are expensive!

Better forget details? Fluid approaches are very convenient!

Magnetohydrodynamics (MHD)

- Fluid plasma model in which the magnetic field $\mathbf{B}$ is 'frozen in':

$$\partial_t(\mathbf{B}\cdot \mathrm{d}\mathbf{S}) + \pounds_{\boldsymbol{u}}(\mathbf{B}\cdot \mathrm{d}\mathbf{S}) = 0\,, \quad \text{or, equivalently,} \quad \partial_t \mathbf{B} + \nabla\times(\mathbf{B}\times\boldsymbol{u}) = 0$$

  Here, $\mathbf{B}\cdot\mathrm{d}\mathbf{S}$ is a differential 2-form and $\pounds_{\boldsymbol{u}}$ denotes Lie derivative.

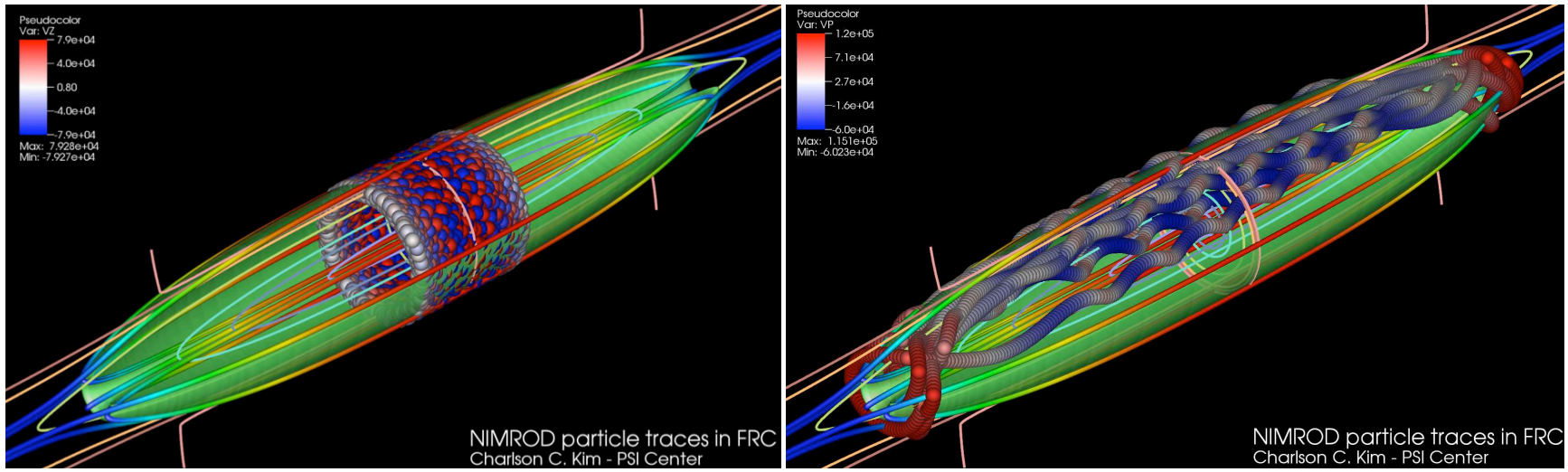
- Fluid equation is [Alfvén (1942)]

$$\frac{\partial \boldsymbol{u}}{\partial t} + (\boldsymbol{u}\cdot\nabla)\boldsymbol{u} = -\frac{1}{\rho}\nabla \mathrm{p} - \frac{1}{\mu_0\rho}\mathbf{B}\times\nabla\times\mathbf{B}$$

  where ρ is the transported mass density and p denotes pressure

- This is a Lie-Poisson Hamiltonian model! [Morrison&Greene('80)]

Still, energetic particles require kinetic theory!



Hot particle dynamics in (Pressure-Coupling) hybrid simulations (NIMROD code) for Field Reversed Configuration experiments (FRCs). *Right*: low energy particles colored by poloidal velocity. *Left*: high energy particles colored by axial velocity. Hot particles confine to the outboard region (higher magnetic gradients) and never cross the origin. *(Figure by the Plasma Science and Innovation Center, University of Washington).*

Kinetic theory & electromagnetism: Maxwell-Vlasov

- Vlasov kinetic equation for $f(\mathbf{x}, \mathbf{p}, t)\ldots$

$$\frac{\partial f}{\partial t} + \frac{\mathbf{p}}{m} \cdot \frac{\partial f}{\partial \mathbf{x}} + q\left(\mathbf{E} + \frac{\mathbf{p}}{m} \times \mathbf{B}\right) \cdot \frac{\partial f}{\partial \mathbf{p}} = 0$$

- $\ldots$ coupled to Maxwell's equations

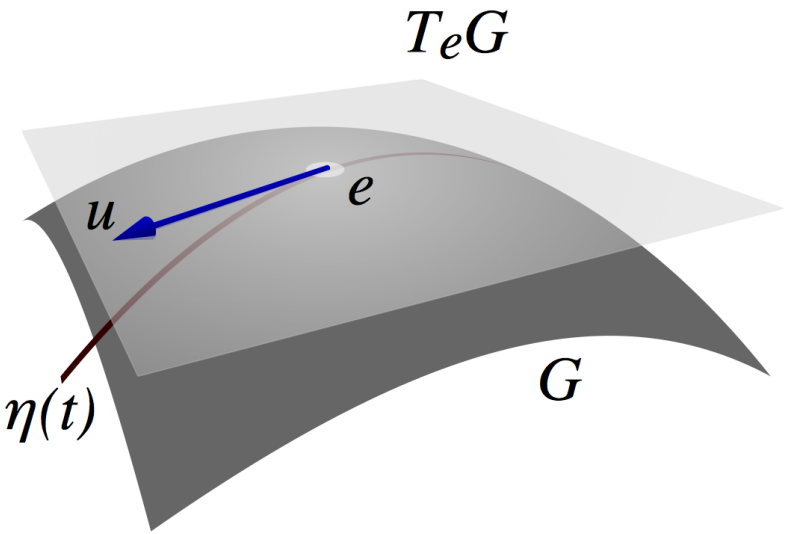
$$\epsilon_0 \mu_0 \frac{\partial \mathbf{E}}{\partial t} = \nabla \times \mathbf{B} - \mu_0 \frac{q}{m} \int \mathbf{p}\, f \, \mathrm{d}^3\mathbf{p}$$

$$\frac{\partial \mathbf{B}}{\partial t} = -\nabla \times \mathbf{E}$$

$$\epsilon_0 \nabla \cdot \mathbf{E} = q \int f \, \mathrm{d}^3\mathbf{p}\,, \qquad \nabla \cdot \mathbf{B} = 0$$

- This is also a Lie-Poisson system! [Morrison('80), Marsden&Weinstein('82)]

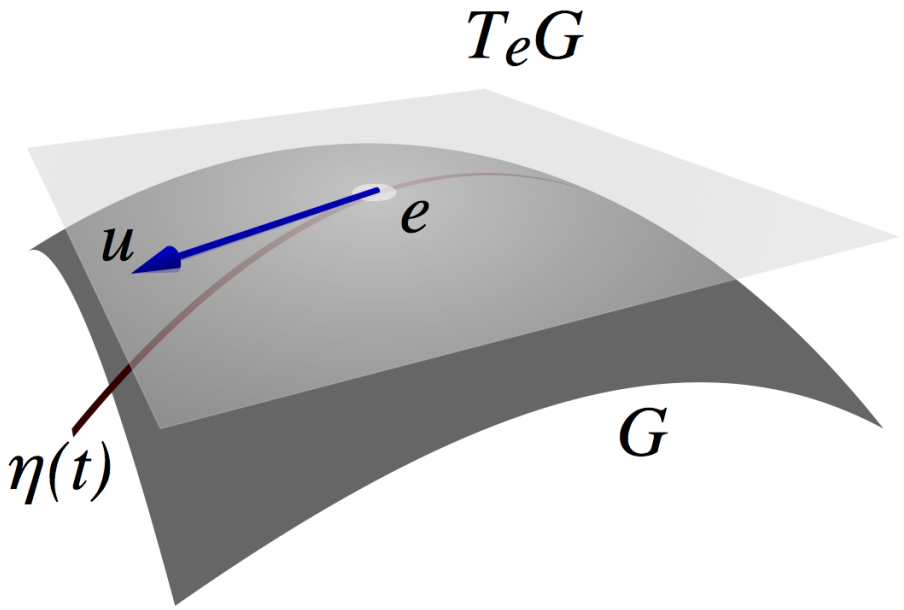
Geometric continuum dynamics



Lagrangian and Eulerian variables are related by the relabeling symmetry, which produces an *intrinsic geometric description* [Arnold (1966)] capturing essential features such as *circulation laws* and dynamical invariants.

Ex. Incompressible ideal fluids move along geodesics on $G = \mathrm{Diff}_{\mathrm{vol}}(M)$

Geometric approach based on variational and Hamiltonian formulations!



Lagrangian fluid dynamics of $\eta(\mathbf{a}, t)$ on the Lie group G possesses the

canonical Poisson bracket: $\{F, G\} = \int \left(\frac{\delta F}{\delta \eta} \cdot \frac{\delta G}{\delta \psi} - \frac{\delta F}{\delta \psi} \cdot \frac{\delta G}{\delta \eta} \right) \mathrm{d}^3\mathbf{a}\,,$

Eulerian dynamics on the (dual) tangent space at identity possesses the

Lie-Poisson bracket (symmetry) : $\{F, G\}(\boldsymbol{\sigma}) = \left\langle \boldsymbol{\sigma}, \left[\frac{\delta F}{\delta \boldsymbol{\sigma}}, \frac{\delta G}{\delta \boldsymbol{\sigma}} \right] \right\rangle$

Fluids: (η, ψ) *are Lagrangian coordinates, while* $\boldsymbol{\sigma} =$ *fluid momentum* $\mathbf{m}$.

Vlasov: (η, ψ) *are Lagrangian coordinates, while* $\sigma =$ *distribution function* f.

Lie-Poisson reduction: $\boldsymbol{\sigma} = \boldsymbol{\sigma}(\eta, \psi)$ *is a momentum map*

Momentum maps are everywhere in mechanics

- Rotational symmetry for vectors (*rigid body motion*):

$$[\mathbf{g},\mathbf{k}] = \mathbf{g}\times\mathbf{k} \;\rightarrow\; \{F,G\} = \boldsymbol{\mu}\cdot\frac{\mathrm{d}F}{\mathrm{d}\boldsymbol{\mu}}\times\frac{\mathrm{d}G}{\mathrm{d}\boldsymbol{\mu}}$$

- Relabeling symmetry for velocities (*Euler fluid dynamics*):

$$[\mathbf{v},\mathbf{u}] = (\mathbf{v}\cdot\nabla)\mathbf{u} - (\mathbf{u}\cdot\nabla)\mathbf{v} \;\rightarrow\; \{F,G\} = \int\boldsymbol{\mu}(\mathbf{x})\cdot\left[\frac{\delta F}{\delta\boldsymbol{\mu}},\frac{\delta G}{\delta\boldsymbol{\mu}}\right]\mathrm{d}^3\mathbf{x}$$

- Unitary symmetry for matrix operators (*quantum dynamics*):

$$[A,B] = AB - BA \;\rightarrow\; \{F,G\} = \hbar\,\mathsf{Tr}\left(i\rho\left[\frac{\delta F}{\delta\rho},\frac{\delta G}{\delta\rho}\right]\right)$$

- Canonical symmetry for phase-space functions (**Vlasov equation**):

$$[h,k] = \frac{\partial h}{\partial\mathbf{x}}\cdot\frac{\partial k}{\partial\mathbf{p}} - \frac{\partial h}{\partial\mathbf{p}}\cdot\frac{\partial k}{\partial\mathbf{x}} \;\rightarrow\; \{F,G\} = \int f(\mathbf{x},\mathbf{p})\left[\frac{\delta F}{\delta f},\frac{\delta G}{\delta f}\right]\mathrm{d}^3\mathbf{x}\,\mathrm{d}^3\mathbf{p}$$

Let's apply geometric mechanics to formulate hybrid models!

$\rightarrow$ *MHD fluid models need to be coupled to Vlasov-like equations*

A geometric hybrid model: assumptions

- Consider a plasma of a fluid (MHD) bulk and an energetic component
- Express the dynamics in terms of the total momentum $\mathbf{M} = \mathbf{m} + \mathbf{K}$, where $\mathbf{m} = \rho \boldsymbol{u}$ and $\mathbf{K} = \int \mathbf{p} f \, \mathrm{d}^3\mathbf{p}$. Then one wants to assume a *rarefied energetic component* so that $\mathbf{K}$-contributions can be neglected.
- In plasma literature, one replaces $\partial_t \mathbf{K} \simeq 0$ in the equation for the total momentum $\mathbf{M}$. *This breaks Hamiltonian structure: no energy balance!*
- The geometric Hamiltonian approach neglects $\mathbf{K}$-contributions by replacing $\mathbf{m} \simeq \mathbf{M}$ in the Hamiltonian, which is then given by [T(2010)]

$$H = \frac{1}{2} \int \frac{|\mathbf{m}|^2}{\rho} \, \mathrm{d}^3\mathbf{x} + \frac{1}{2\mathrm{m}_h} \int f \, |\mathbf{p}|^2 \, \mathrm{d}^3\mathbf{x} \, \mathrm{d}^3\mathbf{p} + \int \rho \, \mathcal{U}(\rho) \, \mathrm{d}^3\mathbf{x} + \frac{1}{2\mu_0} \int |\mathbf{B}|^2 \, \mathrm{d}^3\mathbf{x} \, ,$$

A geometric hybrid model: equations

- This process returns the same fluid equation as in the literature while inserting new transport term and inertial forces [T. (2010)]

$$\frac{\partial \boldsymbol{u}}{\partial t} + (\boldsymbol{u}\cdot\nabla)\boldsymbol{u} = -\frac{1}{\rho}\nabla \mathrm{p} - \frac{1}{\mathrm{m}_h\,\rho}\,\nabla\cdot\int \mathbf{p}\mathbf{p} f\,\mathrm{d}^3\mathbf{p} - \frac{1}{\mu_0\rho}\mathbf{B}\times\nabla\times\mathbf{B}$$

$$\frac{\partial f}{\partial t} + \left(\frac{\mathbf{p}}{m_h} + \boldsymbol{u}\right)\cdot\frac{\partial f}{\partial \mathbf{x}} + \left[q_h\mathbf{E} - \nabla(\mathbf{p}\cdot\boldsymbol{u}) + q_h\left(\frac{\mathbf{p}}{m_h} + \boldsymbol{u}\right)\times\mathbf{B}\right]\cdot\frac{\partial f}{\partial \mathbf{p}} = 0$$

$$\frac{\partial \rho}{\partial t} + \nabla\cdot(\rho\,\boldsymbol{u}) = 0\,, \qquad \frac{\partial \mathbf{B}}{\partial t} = -\nabla\times\mathbf{E}\,, \qquad \mathbf{E} = -\boldsymbol{u}\times\mathbf{B}\,,$$

- Inertial forces – particles now move in the (Lagrangian) fluid frame.

- Dropping $\boldsymbol{u}$ in 2nd eqn yields the non-Hamiltonian model [Park&*al*('92)]

- Helicity invariants [Holm, T. (2012); T, Tassi & Morrison (2015)]:

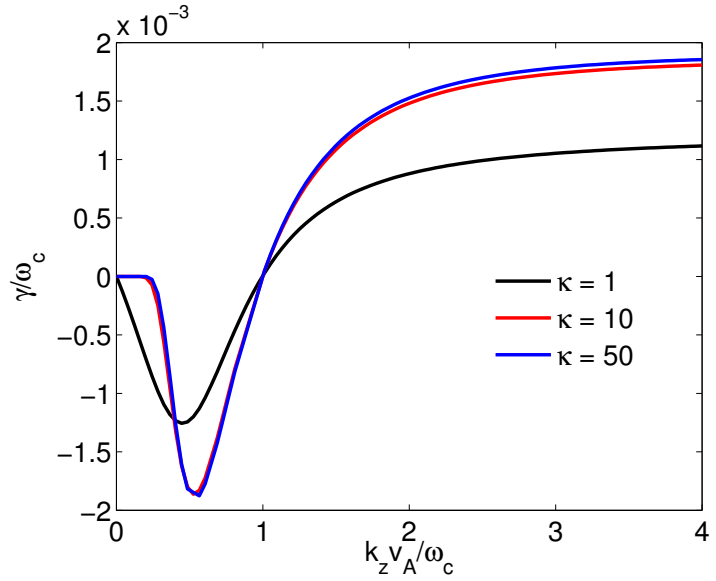
$$\mathcal{H} = \int \mathbf{A}\cdot\mathbf{B}\,\mathrm{d}^3\mathbf{x}\,, \qquad \Lambda = \int\left(\boldsymbol{u} - m_h\frac{\mathbf{K}}{\rho}\right)\cdot\mathbf{B}\,\mathrm{d}^3\mathbf{x}$$

Static equilibria – magnetized Landau damping

Linearize around static $\kappa-$equilibria with $f_0 = f_0(p^2/2)$ and define $F = \int f_0 \, \mathrm{d}^2\mathbf{p}_\perp$. For longitudinal propagation, one obtains (with $v_A = b/\sqrt{\mu_0}$)

$$\omega^2 - k_z^2 v_A^2 + \omega\left(\alpha\omega \mp \omega_c\right)\left(n_0 + \left(\omega \mp \omega_c\right)\int_{-\infty}^{+\infty} \frac{F \, \mathrm{d}p_z}{k_z p_z - \omega \pm \omega_c}\right) = 0.$$

Old hybrid model – growth rate



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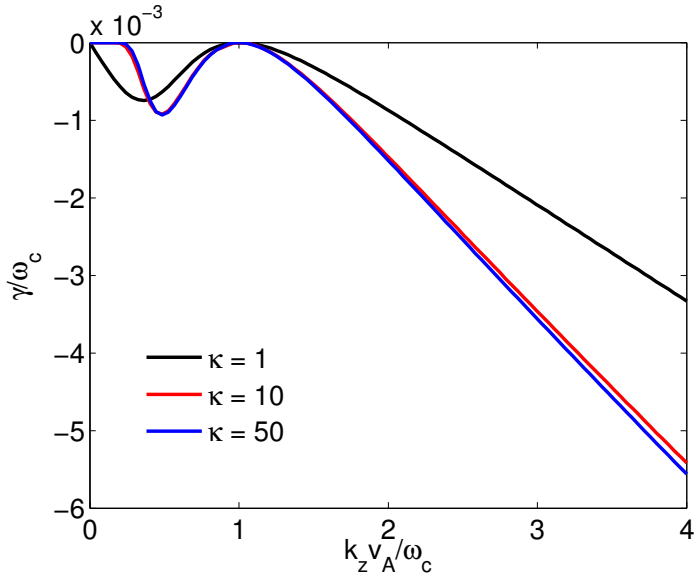

New model ($\alpha = 1$) gives magnetized kinetic damping

Spurious instability in the non-Hamiltonian model! ($\alpha = 0$)

[T, Tassi, Camporeale & Morrison (2014)]

Where's the geometry? Semidirect products!

- The momentum shift $\mathbf{M} = \rho\boldsymbol{u} + \mathbf{K}$ corresponds to a *Poisson diffeomorphism* [Krishnaprasad & Marsden (1984)]

$$\mathcal{E} : \Big(\mathfrak{x}(\mathbb{R}^3) \oplus \mathfrak{x}_{\mathsf{Ham}}(\mathbb{R}^6)\Big)^* \to \Big(\mathfrak{x}(\mathbb{R}^3) \circledS\, \mathfrak{x}_{\mathsf{Ham}}(\mathbb{R}^6)\Big)^*$$
$$(\rho\boldsymbol{u}, \mathbf{K}) \mapsto (\rho\boldsymbol{u} + \mathbf{K}, \mathbf{K})$$

- Denote two-forms by $\Omega^2(\mathbb{R}^3)$. Hybrid model is Lie-Poisson on the Lie group

$$\underbrace{\Big(\mathsf{Diff}(\mathbb{R}^3) \circledS\, \mathsf{Diff}_{\mathsf{Ham}}(\mathbb{R}^6)\Big)}_{\text{cold \& hot flows (Lagrangian paths)}} \circledS \underbrace{\Big(C^\infty(\mathbb{R}^3) \times \Omega^2(\mathbb{R}^3)\Big)}_{\text{dual to advected quantities: } (\rho, \mathbf{A})}$$

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- Semidirect-product arises from *cotangent-lifts of* $\mathsf{Diff}_{Ham}(\mathbb{R}^3)$ *acting on* $\mathsf{Diff}(\mathbb{R}^6)$ *(subgroup action)*, whose **equivariant momentum map** is

$$f(\mathbf{x}, \mathbf{p}) \mapsto \int \mathbf{p}\, f(\mathbf{x}, \mathbf{p})\, \mathrm{d}^3\mathbf{p} = \mathbf{K}(\mathbf{x})$$

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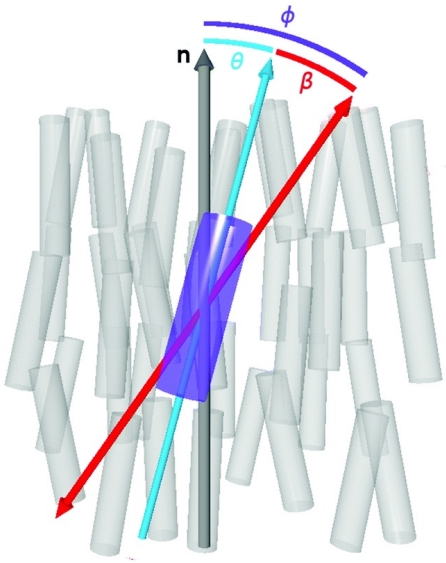
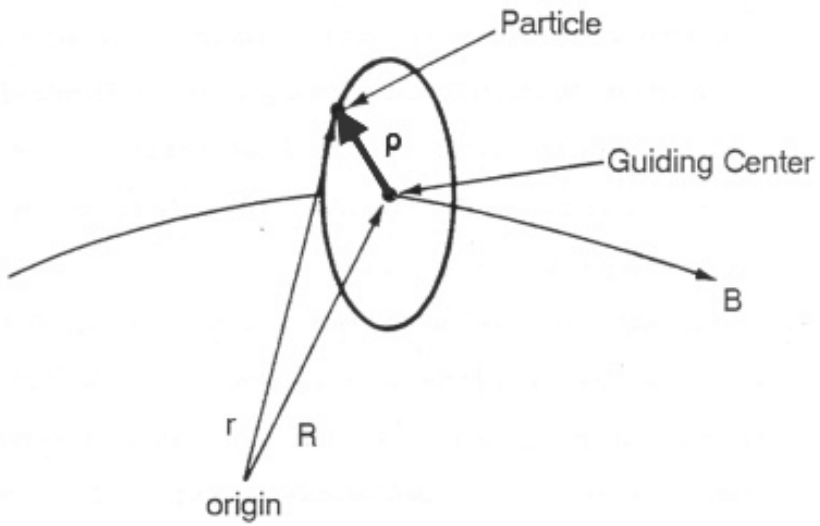
- We confused $\mathsf{Diff}_{\mathsf{Ham}}(\mathbb{R}^3)$ with its extension $\mathsf{Diff}_{\mathsf{Ham}}(\mathbb{R}^3) \times \mathbb{R}$ *(see later)*

Guiding-center (GC) motion: analogy with liquid crystals





- In liquid crystals, rod-like molecules move carrying an orientation, i.e. a **rotational field** $\mathcal{R}(\boldsymbol{x},t)\in SO(3)$ [Gay-Balmaz, Ratiu & T ('13)]

- Locally, molecules align along a certain direction called **director field**

$$\mathbf{n}(\boldsymbol{x},t)=\mathcal{R}(\boldsymbol{x},t)\mathbf{n}_0(\boldsymbol{x})\,,\qquad \partial_i\mathbf{n}(\boldsymbol{x},t)=-\boldsymbol{\gamma}_i(\boldsymbol{x},t)\times\mathbf{n}(\boldsymbol{x},t)$$

where $\gamma=\gamma_i^a(\boldsymbol{x},t)\,\mathrm{d}x^i\mathbf{e}_a$ is a **rotational strain** (*topological defects*).

- Littlejohn's GC theory (to 1st order) has a similar formulation [T ('16)]:

$$\boldsymbol{\rho}(\boldsymbol{x},t)=\rho(t)\mathcal{R}(\boldsymbol{x},t)\boldsymbol{a}_0(\boldsymbol{x})\,,\qquad \mathcal{R}(\boldsymbol{x},t)=e^{-\Theta(t)\widehat{b}(\boldsymbol{x},t)/\varepsilon}$$

where $\widehat{b}_{jk}=-\epsilon_{jkl}b_l$ identifies the magnetic field direction $\boldsymbol{b}=\mathbf{B}/B$.

Guiding-center hybrid-MHD

Alex Close's PhD thesis:

$$\rho\left(\frac{\partial}{\partial t}+\boldsymbol{U}\cdot\nabla\right)\boldsymbol{U}=-\nabla \mathsf{p}-\frac{1}{\mathsf{m}_h}\,\nabla\cdot\mathbb{P}-\frac{1}{\mu_0}\mathbf{B}\times\nabla\times\mathbf{B}$$

$$\frac{\partial\rho}{\partial t}+\nabla\cdot(\rho\boldsymbol{U})=0\,,\qquad \frac{\partial f}{\partial t}+\nabla\cdot(f\boldsymbol{\mathcal{X}})=0$$

$$\frac{\partial\mathbf{B}}{\partial t}=-\nabla\times\mathbf{E}\,,\qquad \mathbf{E}=-\boldsymbol{U}\times\mathbf{B}\,,$$

where $\boldsymbol{\mathcal{X}}(\mathbf{x},v_\parallel)=(\mathbf{u}(\mathbf{x},v_\parallel),a_\parallel(\mathbf{x},v_\parallel))$ and $\mathbb{P}(\mathbf{x},t)$ are given by

$$\boldsymbol{\mathcal{X}}=\left(\frac{\mathbf{B}^*}{B_\parallel^*}(v_\parallel+U_\parallel)-\frac{\mathbf{b}}{B_\parallel^*}\times\Big(a_h\mathbf{E}^*-\nabla(v_\parallel U_\parallel)\Big)\,,\ \frac{\mathbf{B}^*}{B_\parallel^*}\cdot\Big[a_h\mathbf{E}^*-\nabla(v_\parallel U_\parallel)\Big]\right)$$

$$\mathbb{P}=\int f\Big[\underbrace{v_\parallel(\mathbf{u}-\boldsymbol{U})_\perp\mathbf{b}^T+v_\parallel\mathbf{b}(\mathbf{u}-\boldsymbol{U})_\perp^T}_{\textit{new stress terms}}+\underbrace{v_\parallel^2\mathbf{b}\mathbf{b}^T+\mu B(\mathbf{1}-\mathbf{b}\mathbf{b}^T)}_{\textit{'usual' CGL pressure tensor}}\Big]\,\mathrm{d}\mu\,\mathrm{d}v_\parallel$$

- When $\boldsymbol{U}=0$, $\mathbb{P}$ reduces to the newly found GC stress tensor [Brizard&T('16)]
- Variational formulation contains a lot of geometry! [Close, Burby & T ('18)]

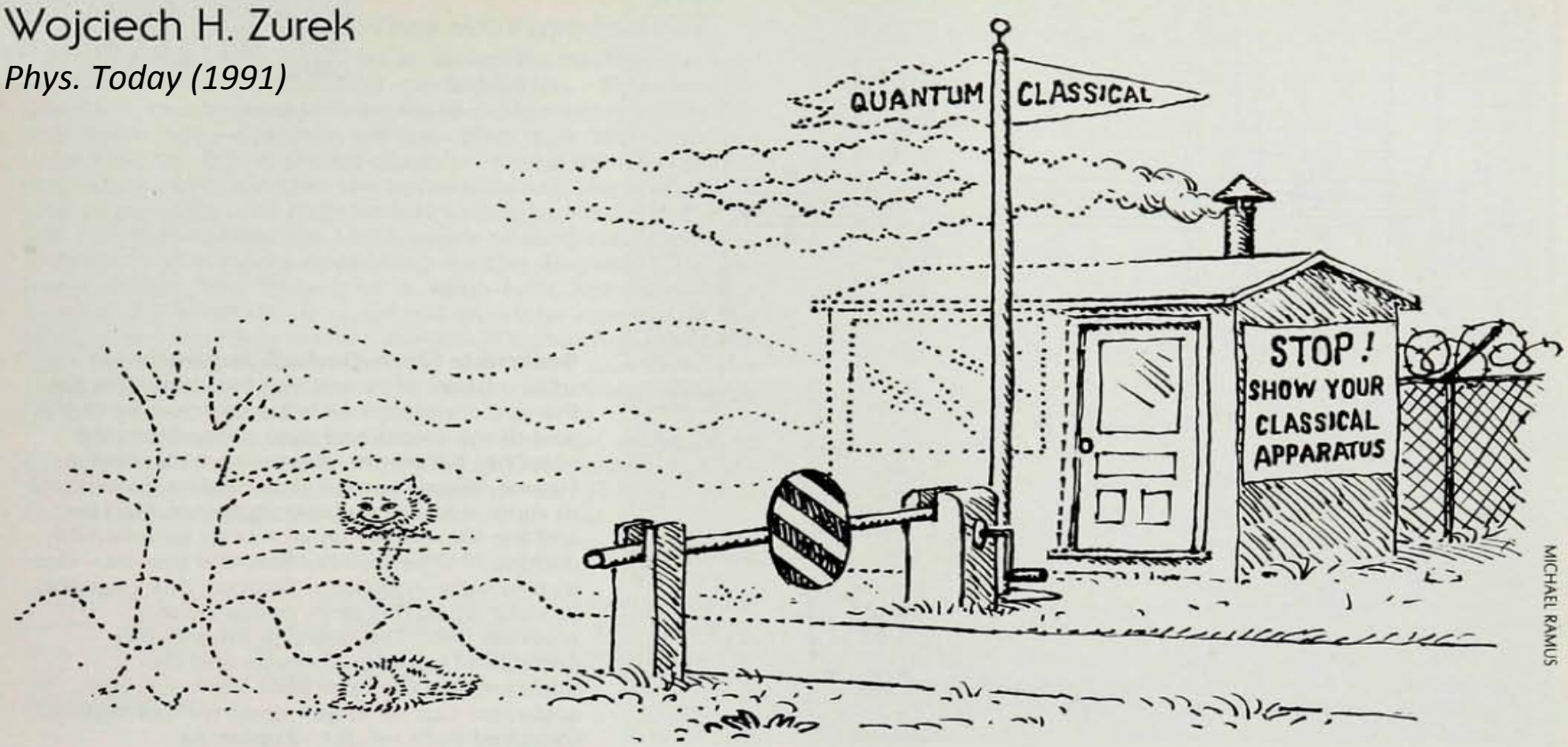
First message:

to derive reduced models, it's better (if possible) to **insert the approximations in the Hamiltonian/Lagrangian** than in the eqns of motion!

Geometric approach to hybrid classical-quantum systems

Wojciech H. Zurek

Phys. Today (1991)



Delineating the border between the quantum realm ruled by the Schrödinger equation and the classical realm ruled by Newton's laws is one of the unresolved problems of physics. **Figure 1**

The search for classical-quantum coupling

Since the raise of quantum mechanics, classical-quantum coupling has emerged as an outstanding question in

- **Quantum measurement theory:** when a quantum state is measured, it undergoes an interaction with a *classical apparatus*
- **Chemical physics:** necessity of approximating the nuclei as classical objects interacting with an electron ensemble

After about a century of continuing efforts, what do we know?

- When a quantum state interacts with a classical system, the latter undergoes an **uncontrollable disturbance**. (*cf. N. Bohr*)
- When a quantum state interacts with a classical system, the former undergoes **decoherence** (lack of pure state solutions).

NOT MUCH! – *Let's revise both quantum and classical mechanics...*

Quantum & classical states [Chernoff & Marsden (1976)]

- **Quantum pure states**: normalized L^2-functions (ie. $\int |\psi(x)|^2 \, \mathrm{d}x = 1$)

  Schrödinger's equation: $\boxed{i\hbar \, \partial_t \psi = \hat{H} \psi}$

- **Quantum mixed states** are positive-definite operators $\hat{\rho}$ with $\mathrm{Tr}\, \hat{\rho} = 1$:

  von Neumann equation: $\boxed{i\hbar \, \partial_t \hat{\rho} = [\hat{H}, \hat{\rho}]\,,}$

  where $[\cdot, \cdot]$ is the commutator. (Setting $\hat{\rho} = \psi\psi^\dagger$ yields pure states).

- **Classical pure (particle) states** are points in phase-space

  Hamilton's equations for (q, p)*:* $\boxed{\dot{q} = \dfrac{\partial H}{\partial p}\,, \quad \dot{p} = -\dfrac{\partial H}{\partial q}}$

- **Classical mixed states**: positive-definite densities with $\int \rho(q, p) \, \mathrm{d}q\mathrm{d}p = 1$:

  Liouville (Vlasov) equation: $\boxed{\partial_t \rho = \{H, \rho\}}$

  where $\{f, g\} = \partial_q f \partial_p g - \partial_p f \partial_q g$ is the canonical Poisson bracket.
  (Setting $\rho(\mathrm{q}, \mathrm{p}, t) = \delta(\mathrm{q} - q(t))\delta(\mathrm{p} - p(t))$ yields pure states).

Objective:

Hamiltonian *model for interacting classical and quantum particles.*

Ideally, we want to construct a hybrid density

$$\hat{\rho} \otimes \rho(q,p) \longrightarrow \hat{\rho}(q,p)$$

More difficult than kinetic-fluid, where particles and fluid evolve separately.

Two possible strategies for Hamiltonian hybrids

1. **Write quantum states in terms of (Liouville-like) probability densities**

   - The **Wigner-Moyal formalism** $\psi(x) \mapsto W_\psi(x,p)$ provides a description of quantum mechanics in terms of phase-space densities

   - Approach widely studied. Its **Hamiltonian setting is noncanonical** [Bialynicki-Birula & Morrison ('91)], thus leading to complications

2. **Write classical mechanics in terms of (Schrödinger-like) wavefunctions**

   - Following **Koopman's work**, this was proposed in [Sudarshan (1976)]

   - This approach seems promising because wavefunctions have a **simple (canonical) Hamiltonian** setting $\rightarrow$ important simplification

. . . Second method leads to interpretative problems – can we solve those?

The Koopman-von Neumann equation

Question: can we define an L^2-function $\Psi(q,p)$ such that the probability density $\rho = |\Psi|^2$ satisfies the classical Liouville equation $\partial_t \rho = \{H, \rho\}$?

Theorem (adapted from [Koopman, 1931]). Let $H(q,p)$ be a phase-space function and let $\Psi \in L^2(\mathbb{R}^2)$ satisfy the

KvN equation $\boxed{i\hbar\, \partial_t \Psi = \{i\hbar H, \Psi\}}$

Then $\rho = |\Psi|^2$ satisfies $\partial_t \rho = \{H, \rho\}$. *(See also [von Neumann (1932)]).*

The Hermitian (self-adjoint) operator $\hat{L}_H := \{i\hbar H, \_\,\}$ is called the **Liouvillian**

$$i\hbar\, \partial_t \Psi = \hat{L}_H \Psi$$

Sudarshan extended KvN to include the interaction with quantum degrees of freedom: *hybrid wavefunction* $\Psi(q,p) \otimes \psi(x) \to \Upsilon(q,p,x)$.

However, by invoking superselection rules for physical consistency, Sudarshan's (Hamiltonian!) theory leads to fundamental interpretative issues.

Hamiltonian structure of the KvN equation

The KvN eqn. possesses the standard (canonical) variational principle (VP):

$$\boxed{\delta \int_{t_1}^{t_2} \int \left(\hbar \,\mathrm{Re}(i\Psi^* \partial_t \Psi) - \Psi^* \hat{L}_H \Psi \right) \mathrm{d}q\mathrm{d}p \; \mathrm{d}t = 0 \,,}$$

Remarks:

- Conserved energy: $\int \Psi^* \hat{L}_H \Psi \, \mathrm{d}q\mathrm{d}p = \hbar \int H \, \mathrm{Im}\{\Psi, \Psi^*\} \, \mathrm{d}q\mathrm{d}p = \mathrm{const}\,.$

  This is **different from the physical energy** $\int \rho H \, \mathrm{d}q\mathrm{d}p = \int |\Psi|^2 H \, \mathrm{d}q\mathrm{d}p$ (which is also conserved). Interpretative issue of the KvN formula $\rho = |\Psi|^2$

- $\hat{L}_H$ is **not unique**: the correspondence $H \mapsto \{i\hbar H, \_\}$ is many-to-one

- **More fundamental issue**: the integrand in the VP does not transform consistently under gauge transformations $\Psi(q,p) \mapsto e^{iS(q,p)} \Psi(q,p)$

  Classical gauge covariance (equivariance) is violated

Claim: **the Koopman-von Neumann theory is incomplete.**

Canonical transformations and their central extension

- **Group theory**: $\hat{L}_H := \{i\hbar H, \_\}$ generates **canonical transformations**

$$(q,p) \mapsto \Big(Q(q,p), P(q,p)\Big), \qquad (Q,P) \in \mathsf{Diff}_{\mathsf{Ham}}(\mathbb{R}^2)$$

- In classical mechanics, one says that **the Hamiltonian function** H **generates the dynamics** (Hamiltonian flow) by Hamilton's equations.

- However, **Hamiltonians are only defined up to constants**: H and $H' = H + \kappa$ generate the same dynamics!

- **Van Hove (1951)**: don't look at $\mathsf{Diff}_{\mathsf{Ham}}(\mathbb{R}^2)$, but rather look at the **central extension** $\mathsf{Diff}_{\mathsf{Ham}}(\mathbb{R}^2) \times \mathbb{R}$ (*strict contact transformations*)

  Product rule: $$(\eta_1,\kappa_1)(\eta_2,\kappa_2) = \left(\eta_1 \circ \eta_2,\ \kappa_1+\kappa_2+\int_0^{\eta_2(0)} (\eta_1^* \mathcal{A} - \mathcal{A})\right)$$

  Here, $\circ$ denotes composition, $*$ denotes pullback, and $\mathcal{A} = (q\mathrm{d}p - p\mathrm{d}q)/2$.

  $\rightarrow$ *The Lie algebra coincides with the Poisson algebra* $(C^\infty(\mathbb{R}^2), \{\cdot,\cdot\})$

Modifying the Louvillian: prequantum operator

Theorem [Van Hove, 1951]. Strict contactomorphisms carry the following (right) **unitary representation** on $L^2(\mathbb{R}^2)$ (denote $\mathbf{z} = (q, p)$):

$$\Psi(\mathbf{z}) \mapsto e^{i\hbar^{-1}\left(\kappa + \int_0^{\mathbf{z}} (\eta^* \mathcal{A} - \mathcal{A})\right)} (\eta^* \Psi),$$

whose infinitesimal generator is given by $i\hbar^{-1}\hat{\mathcal{L}}_H$, where

$$\hat{\mathcal{L}}_H = \hat{L}_H - \underbrace{\left(\frac{1}{2}\mathbf{z} \cdot \nabla_{\mathbf{z}} H - H\right)}_{\text{Lagrangian!}}. \quad (H \mapsto \hat{\mathcal{L}}_H \textit{ is one-to-one: uniqueness!})$$

There's a whole lot of geometry here! In **geometric quantization** (*prequantization*), the modified Liouvillian $\hat{\mathcal{L}}_H$ is called *prequantum operator:*

Lie algebra structure: $$[\hat{\mathcal{L}}_H, \hat{\mathcal{L}}_K] = i\hbar \hat{\mathcal{L}}_{\{H,K\}}$$

Given a function $A(\mathbf{z})$, the map $A(\mathbf{z}) \to i\hbar^{-1}\widehat{\mathcal{L}}_A$ is a **Lie Algebra isomorphism**

Modifying the Koopman-von Neumann theory

Now, we perform the replacement $\hat{L}_H \to \hat{\mathcal{L}}_H$ in KvN theory:

- KvN equation becomes $i\hbar\,\partial_t\Psi = \hat{\mathcal{L}}_H\Psi$ (notice: $\hbar$ no longer cancels!)

- The KvN variational principle becomes gauge-covariant (equivariant):

$$\delta \int_{t_1}^{t_2} \int \Big(\hbar\,\mathrm{Re}(i\Psi^*\partial_t\Psi) - \Psi^*\hat{\mathcal{L}}_H\Psi \Big)\, \mathrm{d}^2z\ \mathrm{d}t = 0\,,$$

- Conserved energy: $\int \Psi^*\hat{\mathcal{L}}_H\Psi\,\mathrm{d}^2z = \int H\Big(|\Psi|^2 + \mathrm{div}\,\mathcal{J}\Big)\,\mathrm{d}^2z$ with

$$\mathcal{J} = \frac{1}{2}\mathbf{z}|\Psi|^2 + i\hbar\Psi^*\mathbb{J}\nabla\Psi\,, \qquad \text{with} \quad \mathbb{J} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$$

$\to$ *What's the meaning of the quantity* $|\Psi|^2 + \mathrm{div}\,\mathcal{J}$*?*

The quantity $|\Psi|^2 + \operatorname{div} \mathcal{J}$

Answer [Gay-Balmaz, T (2018)]: The map

$$J : \Psi \mapsto |\Psi|^2 + \operatorname{div} \mathcal{J}$$

is a **MOMENTUM MAP** for the action of strict contacto's on $L^2(\mathbb{R}^2)$, that is it satisfies

$$\langle A | J(\Psi) \rangle = \frac{1}{2} \Omega(\Psi, i\hbar^{-1} \hat{\mathcal{L}}_A \Psi) \,, \qquad \forall\, A \in C^\infty(\mathbb{R}^2) \,,$$

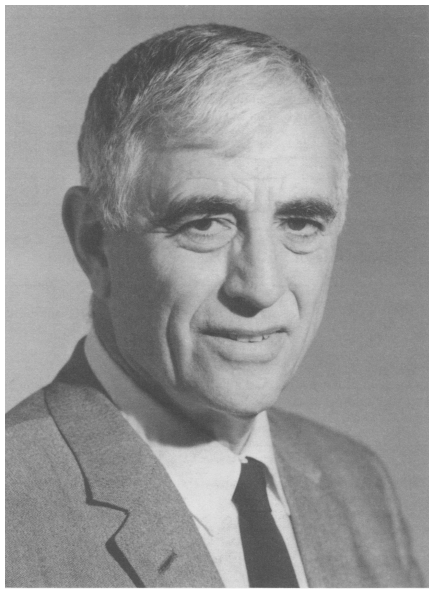
where $\langle \cdot | \cdot \rangle$ is the L^2-inner product and $\Omega(\Psi_1, \Psi_2) = 2\hbar\, \mathbf{Im} \langle \Psi_1 | \Psi_2 \rangle$.

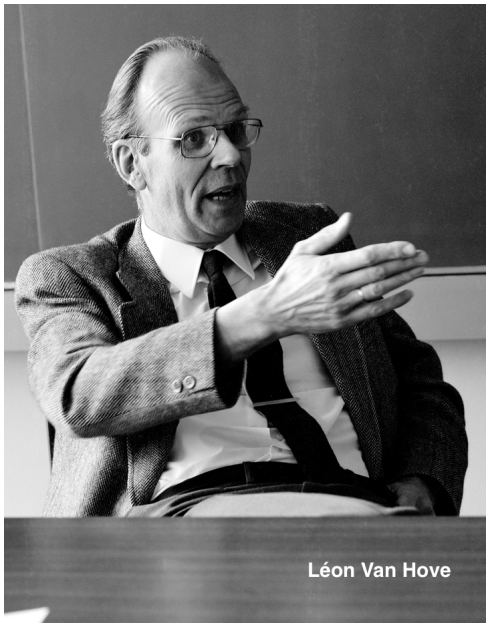
- Setting $\rho = |\Psi|^2 + \operatorname{div} \mathcal{J}$ **returns the Liouville equation** $\partial_t \rho = \{H, \rho\}$
  The sign of ρ is preserved in time: positivity is preserved!

- Notice: $\int \operatorname{div} \mathcal{J} \, \mathrm{d}^2 z = 0 \;\longrightarrow\; \mathcal{J}$ doesn't contribute to total probability!

The quantity $|\Psi|^2 + \operatorname{div} \mathcal{J}$ is a **representation of the classical probability density!**

Recap: Koopman–Van Hove classical mechanics


Bernard Osgood Koopman



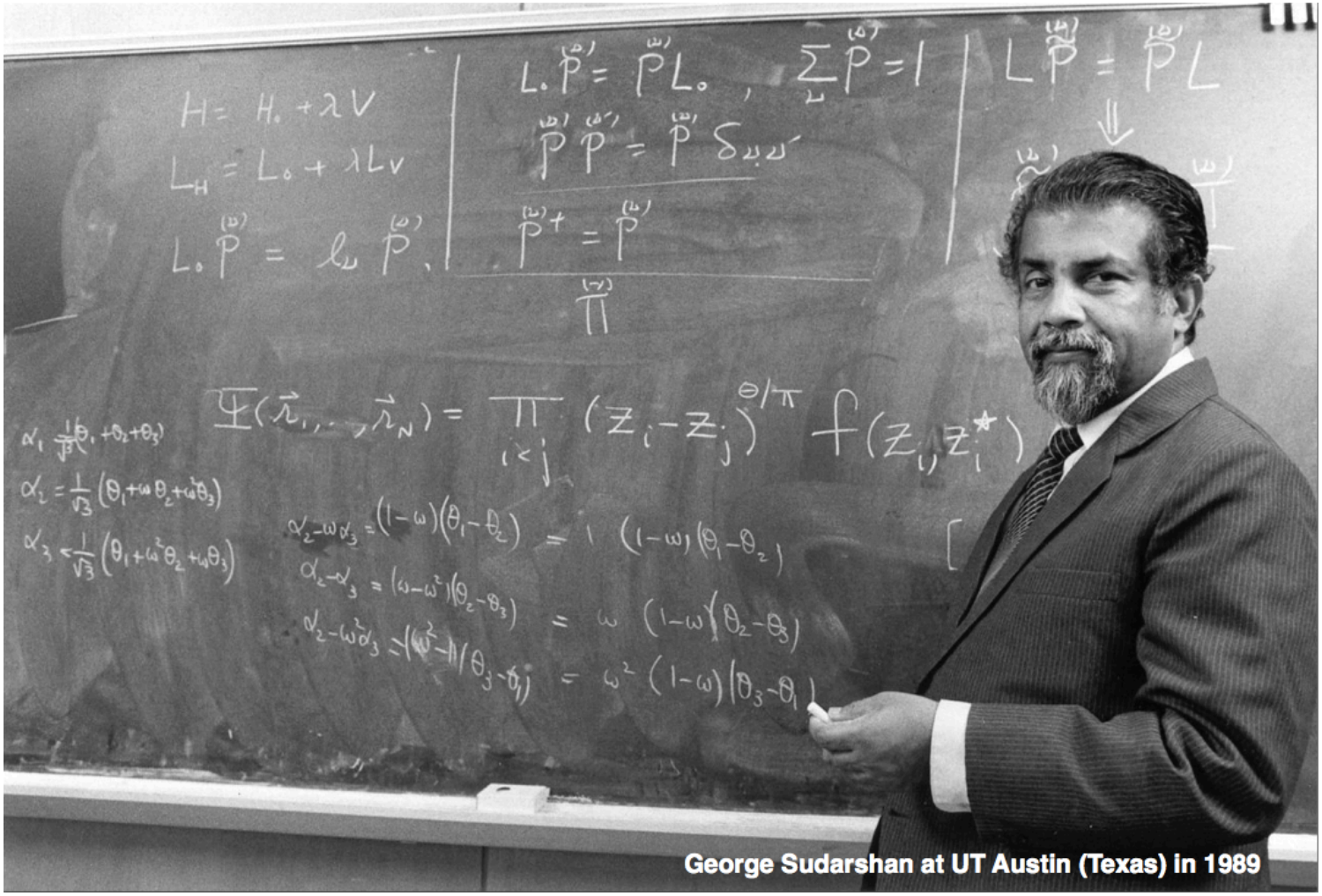
Combining KvN theory with Van Hove's central extension yields the following (Clebsch) representation of the Liouville probability density:

$$\rho = |\Psi|^2 + \hbar\,\mathrm{Im}\{\Psi^*, \Psi\} + \frac{1}{2}\,\mathrm{div}\Big(\mathbf{z}|\Psi|^2\Big)$$

Koopman-van Hove equation (KvH) for the classical wavefunction:

$$i\hbar\frac{\partial\Psi}{\partial t} = \{i\hbar H, \Psi\} - \left(\frac{1}{2}\,\mathbf{z}\cdot\nabla H - H\right)\Psi$$

Let's exploit Shudarshan's idea for classical-quantum hybrids!



In 1976, George Sudarshan (Sep 1931 – May 2018) first proposed the idea of using classical (KvN) wavefunctions for classical-quantum coupling.

However, as we showed, KvN alone is incomplete. *Use Koopman–Van Hove!*

Construction of classical-quantum hybrids

Towards hybrid theories: the quantization process

- There is a well-known procedure taking the Koopman–van Hove equation $i\hbar\,\partial_t\Psi = \hat{\mathcal{L}}_H\Psi$ into the Schrödinger equation $i\hbar\,\partial_t\Psi = \hat{H}\Psi$ (with $\hat{H} = \hat{T} + \hat{V}$, kinetic + potential).

- Upon avoiding technicalities, one sets

$$\partial_p\Psi = 0\,, \qquad\qquad p\Psi = -i\hbar\partial_q\Psi$$

  to obtain $i\hbar\,\partial_t\Psi(q) = [(-i\hbar\partial_q)^2 + V(q)]\Psi(q)$.

- In short: $\Psi(q,p) \longrightarrow \Psi(q)$

- Although this (formal) process is well-known in geometric quantization, it is pretty unknown within the physics community

Caution: *here we focus on the case $H = T + V$.*
However, different methods lead to the same result (not covered here)

Strategy: partial quantization procedure

Write the KvH equation for 2 classical particles and quantize only one!

$$\Upsilon(q, p, x, \sigma) \longrightarrow \Upsilon(q, p, x)$$

The hybrid wave equation

The partial quantization procedure yields the hybrid wavfunction equation

$$i\hbar\frac{\partial\Upsilon}{\partial t} = \{i\hbar\widehat{H},\Upsilon\} - \left(\frac{1}{2}\mathbf{z}\cdot\nabla_{\mathbf{z}}\widehat{H} - \widehat{H}\right)\Upsilon =: \widehat{\mathcal{L}}_{\widehat{H}}\Upsilon\,,$$

where $\mathbf{z} = (q,p)$ and $\widehat{H} = \widehat{H}(\mathbf{z})$ is an **operator-valued function on phase-space**

Equations of the same type were found by Boucher & Traschen in 1988!

However, these equations were rejected since

- they were claimed by the authors to yield *"interpretative difficulties"*
- Also, B&T claimed the absence of a positive conserved energy

On the other hand, by construction the same equation arises from the VP

$$\delta\int_{t_1}^{t_2}\int\left(\hbar\,\mathrm{Re}(i\Upsilon^*\partial_t\Upsilon) - \Upsilon^*\widehat{\mathcal{L}}_{\widehat{H}}\Upsilon\right)\mathrm{d}^2z\,\mathrm{d}x\;\mathrm{d}t = 0\,,$$

$\rightarrow$ The sign of the conserved energy $\int\Upsilon^*\widehat{\mathcal{L}}_{\widehat{H}}\Upsilon\,\mathrm{d}^2z\,\mathrm{d}x$ is preserved in time!

Hybrid probability density

In both classical and quantum mechanics, there exists a density (function $\rho(q,p)$ or operator $\hat{\rho}$) such that the total energy is formally written as

$$\langle \rho | H \rangle \, .$$

The energy is linear in ρ and H. (Here, $\langle \cdot | \cdot \rangle$ denotes the natural inner product).

Question: Can we define a density-like object $\widehat{\mathcal{D}}$ such that

$$\int \Upsilon^* \widehat{\mathcal{L}}_{\widehat{H}} \Upsilon \, \mathrm{d}^2 z \, \mathrm{d}x = \langle \widehat{\mathcal{D}} | \widehat{H} \rangle \, ?$$

Answer: Yes! We have $\int \Upsilon^* \widehat{\mathcal{L}}_{\widehat{H}} \Upsilon \, \mathrm{d}^2 z \, \mathrm{d}x = \mathrm{Tr} \int \widehat{\mathcal{D}}(\mathbf{z}) \, \widehat{H}(\mathbf{z}) \, \mathrm{d}^2 z$, where

$$\boxed{\widehat{\mathcal{D}}(\mathbf{z}) := \Upsilon(\mathbf{z})\Upsilon^\dagger(\mathbf{z}) + i\hbar\{\Upsilon(\mathbf{z}), \Upsilon^\dagger(\mathbf{z})\} + \frac{1}{2}\,\mathrm{div}\Big(\mathbf{z}\Upsilon(\mathbf{z})\Upsilon^\dagger(\mathbf{z})\Big)}$$

More on probability densities: quantum and classical

Question: Fine – we have a hybrid density $\widehat{\mathcal{D}}(\mathbf{z})$, but how do we reconstruct the quantum density operator $\hat{\rho}$ and the classical density $\rho(q,p)$?

Answer: We simply project $\widehat{\mathcal{D}}(\mathbf{z})$ on the quantum density operators and on the classical density functions, respectively:

$$\hat{\rho} = \int \widehat{\mathcal{D}}(\mathbf{z})\, \mathrm{d}^2 z\,, \qquad\qquad \rho(q,p) = \mathrm{Tr}\, \widehat{\mathcal{D}}(\mathbf{z})$$

- Quantum density operator: $\hat{\rho} = \int \Upsilon(\mathbf{z})\Upsilon^\dagger(\mathbf{z})\, \mathrm{d}^2 z \;\rightarrow$ **POSITIVE!**

$\rightarrow$ *Only available hybrid theory capturing positivity of the quantum density!*

- Classical density: $\rho(q,p) = |\Upsilon(\mathbf{z})|^2 - i\hbar\{\Upsilon(\mathbf{z})^\dagger, \Upsilon(\mathbf{z})\} + \frac{1}{2}\,\mathrm{div}(\mathbf{z}|\Upsilon(\mathbf{z})|^2\Big)$

$\rightarrow$ *Lack of classical positivity in hybrid systems was explained by Boucher (1988)*

Dynamics of the hybrid probability density

In 1981, Aleksandrov and Gerasimenko independently proposed an equation for the hybrid density $\widehat{\mathcal{D}}(\mathbf{z})$: the **quantum-classical Liouville equation**

$$\frac{\partial \widehat{\mathcal{D}}}{\partial t} = -i\hbar^{-1}[\widehat{H}, \widehat{\mathcal{D}}] + \frac{1}{2}\Big(\{\widehat{H}, \widehat{\mathcal{D}}\} - \{\widehat{\mathcal{D}}, \widehat{H}\}\Big).$$

Question: We know this is not Hamiltonian, but what's the $\widehat{\mathcal{D}}-$equation resulting from our Hamiltonian construction?

Preliminary question: What do we really know about $\widehat{\mathcal{D}}$?

- The map $\Upsilon\Upsilon^\dagger \mapsto \widehat{\mathcal{D}}$ is the dual of $\widehat{A}(\mathbf{z}) \mapsto \widehat{\mathcal{L}}_{\widehat{A}}$ (**no LA isomorphism!**)
- Unfortunately, $\widehat{\mathcal{D}}$ does not enjoy momentum map properties

$\longrightarrow$ There is no closed equation for $\widehat{\mathcal{D}}$ in the general case!

Answer: An explicit calculation yields **surprising similarities**!

$$\frac{\partial \widehat{\mathcal{D}}}{\partial t} = -i\hbar^{-1}[\widehat{H}, \widehat{\mathcal{D}}] + \Big(\{\widehat{H}, \widehat{\mathcal{D}}\} - \{\widehat{\mathcal{D}}, \widehat{H}\}\Big) + \mathscr{F}(\Upsilon, \nabla\Upsilon)$$

$\mathscr{F}$ is a nasty function: *no closed eqn* (consistent with Salcedo (1999))

Interpretation of the theory: decoherence

From the previous equation for $\widehat{\mathcal{D}}$ (or for Υ), we obtain the dynamics for the quantum and classical probabilities $\hat{\rho} = \int \widehat{\mathcal{D}}(\mathbf{z})\, \mathrm{d}^2 z$ and $\rho(q,p) = \mathrm{Tr}\, \widehat{\mathcal{D}}(\mathbf{z})$:

$$i\hbar \frac{\partial \hat{\rho}}{\partial t} = \int [\widehat{H}, \widehat{\mathcal{D}}]\, \mathrm{d}^2 z\,, \qquad\qquad \frac{\partial \rho}{\partial t} = \mathrm{Tr}\{\widehat{H}, \widehat{\mathcal{D}}\}$$

OK – these are pretty good looking formulas, but what do they mean?

- Pure quantum state solutions $\hat{\rho} = \psi\psi^\dagger$ are no longer preserved in time

  $\rightarrow$ **Absence of pure quantum states $\rightarrow$ Quantum decoherence!**

- Particle-like solutions $\rho(\mathbf{z}, t) = \delta(\mathbf{z} - \boldsymbol{\zeta}(t))$ are also lost

  $\rightarrow$ **Absence of pure classical states $\rightarrow$ 'Classical decoherence'!**

- Generally, sgn$(\rho) \neq$ const: this is explained by using Wigner functions

Second message:

If you have a Hamiltonian theory (e.g. KvN or KvH), look for momentum maps – they will tell you what to do!

That's all – thanks!

Mean-field ansatz: recovering previous theories

Question:

How do we compare with previous theories (mathematically consistent)?

Let us adopt the **mean-field ansatz** (no classical-quantum correlations):

$$\Upsilon(\mathbf{z}, x, t) = \Psi(\mathbf{z}, t)\psi(x, t) \;\rightarrow\; \widehat{\mathcal{D}}(\mathbf{z}, t) = f(\mathbf{z}, t)\,\hat{\rho}(t)$$

with $\hat{\rho} = \psi\psi^{\dagger}$ and $f = |\Psi|^2 + \hbar\,\mathsf{Im}\{\Psi^*, \Psi\} + \mathsf{div}(\mathbf{z}|\Psi|^2)/2$.

Answer: this yields exactly the mean-field model from chemical physics!

$$i\hbar\frac{\partial\hat{\rho}}{\partial t} = \left[\int f\widehat{H}\,\mathsf{d}^2z\,,\hat{\rho}\right], \qquad \frac{\partial f}{\partial t} = \left\{\mathsf{Tr}(\hat{\rho}\widehat{H})\,,f\right\}$$

- The second equation has single-particle solutions $f(\mathbf{z}, t) = \delta(\mathbf{z} - \boldsymbol{\zeta}(t))$

→ *Pure states are recovered in the absence of classical-quantum correlations!*

- Notice that $\mathsf{sgn}(f) = \mathsf{const}$.

→ *Positivity is recovered in the absence of classical-quantum correlations!*

Multi-physics models for hybrid kinetic-fluid and classical-quantum systems - Talk by Cesare Tronci

Lecture notes (Ori S. Katz)

October 15, 2018

Abstract

Many physical situations involve the interplay of different phenomena at different scales. The corresponding description requires the use of multi-physics models, whose mathematical formulation poses several challenges. Examples are found in the classical-quantum coupling in molecular dynamics or in the coupling between mean flow and fluctuation kinetics in turbulence. In plasma physics, the interaction of energetic particles (obeying kinetic theory) with a fluid bulk (obeying magnetohydrodynamics) requires formulating hybrid kinetic-fluid models, which are often obtained by making assumptions that destroy the correct energy balance. This talk shows how momentum-map techniques in geometric mechanics provide a powerful unifying framework for both kinetic-fluid and classical-quantum coupling, thereby leading to new hybrid models in different contexts.

1 Lecture notes

What can you do with a momentum map?

For symplectic maps, the momentum map is known, mostly as a generalization of Noether theorem concerning conserved quantities. We will talk here about momentum maps in the case of non-conserved quantities.

The moment method - starting with kinetic theory on phase space and looking at the moment equations, obtain Euler fluid dynamics equations.

Express particle motion in new frame, obtain a new transport term and inertial forces.

Static equilibria - obtain a new dispersion relation with α. Then, we plotted the growth rate for the old hybrid model and the new hybrid growth rate. In the old hybrid model, we get an instability, but there is no source of energy for this, and the only reason for this spurious instability is because the system does not conserve energy. This convinced us that the new hybrid model is fundamentally different.

Where's the geometry? This momentum shift is a momentum map, corresponding to a Poisson diffeomorphism. The resulting semidirect product arises naturally. There is a momentum map underlying this - the $K(x)$, exactly the term we want to neglect.

Guiding center (GC) motion: analogy with liquid crystals. In liquid crystals, rod-like particles are transported in space, so a rotational field needs to be taken into account as well as a velocity field. It turns out that to the first order, there is an analogy between liquid crystals and guiding center. The director field description of liquid crystals applies to first order Littlejohn's GC theory. The analogy, in a way, is between the physical molecule dragged in space and the particle orientation dragged in space.

GC hybrid-MHD - would like to develop hybrid models in which the energetic particles are approximated by the GC description. Can one build a GC hybrid theory? Yes, but since there is no natural action of the diffeomorphism on the configuration space it is not easy. Need to go to higher dimensions, build the theory there, then project to the 4 dimensional configuration space.

Equations for χ and $\mathbb{P}$: contain the usual pressure tensor and new stress terms. This model was derived by variational methods.

Applying this technique to chemical physics: related to the search for classical-quantum interactions. How to write a hybrid quantum-classical theory? Using the von-Neumann approach to write classical Hamiltonian theory in quantum language by looking at averages (analogous to mixed states in QM) instead of particles (analogous to pure states in QM).

Argument in favor of non-positive classical densities

In QM, different 'pictures' are available: Schrödinger, Heisenberg, Dirac,...
The *phase-space picture* goes back to Wigner (1932) and Moyal (1949)

Wigner transform (LA isomorphism): $\quad \Big(\hat{\rho},\, [\cdot,\cdot]\Big) \mapsto \Big(W_\rho\,, \{\{\cdot,\cdot\}\}\Big)$

$W_\rho\,(q,p)$ is a phase-space function satisfying the **Wigner-Moyal equation**

$$\frac{\partial W_\rho}{\partial t} = \underbrace{\{\{H, W_\rho\}\}}_{\textit{Moyal bracket}} \qquad (\{\{\cdot,\cdot\}\} \textit{ deforms } \{\cdot,\cdot\})$$

- Property 1: W_ρ is **not positive definite**
- Property 2: $\{\{A,B\}\} = \{A,B\}$ if A or B is a **quadratic** function

Consider a harmonic oscillator (coord $\mathbf{z}$) coupled to a nonlinear system (coord $\boldsymbol{\zeta}$): $H(\mathbf{z},\boldsymbol{\zeta})$ *quadratic in* $\mathbf{z}$. WM eqn: $\partial_t W_\rho = \{H, W_\rho\}_{\mathbf{z}} + \{\{H, W_\rho\}\}_{\boldsymbol{\zeta}}$

$$\frac{\partial W_{HO}}{\partial t} = \int \{H, W_\rho\}_{\mathbf{z}}\, \mathrm{d}^2\zeta\,, \qquad \frac{\partial W_{NL}}{\partial t} = \int \{\{H, W_\rho\}\}_{\boldsymbol{\zeta}}\, \mathrm{d}^2 z$$

$\rightarrow$ While W_{HO} is essentially classical, it may become negative because so may W_ρ!

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