Spectral Theory of the Koopman Operator and Fundamentals of Physics

Igor Mezić

Department of Mechanical Engineering & Mathematics, University of California, Santa Barbara

SIAM DS, Snowbird

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Introduction

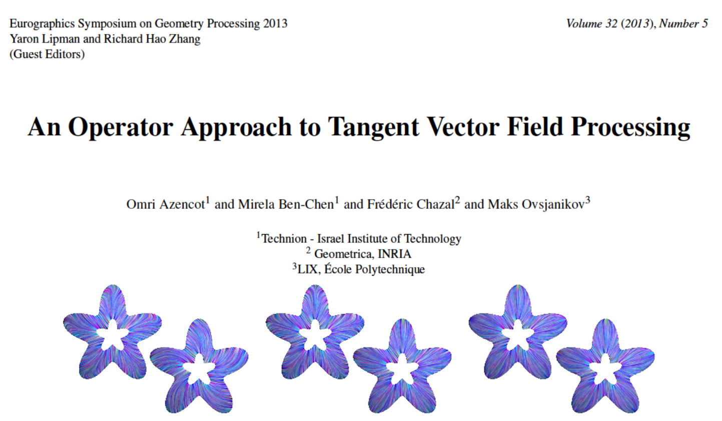
-A reformulation of dynamical systems theory in terms of evolution of observables.

-Koopman and von Neumann used it to study measure-preserving systems.

-Last 20 years; studies of dissipative systems; data-driven methodologies.

-Spectral objects associated with a class of linear, infinite-dimensional, non self-adjoint operators help unravel the state-space geometry and enable model reduction and control in high-dimensional systems.

-Relationship to data analysis is direct: akin to stochastic process theory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An Operator Approach to Tangent Vector Field Processing

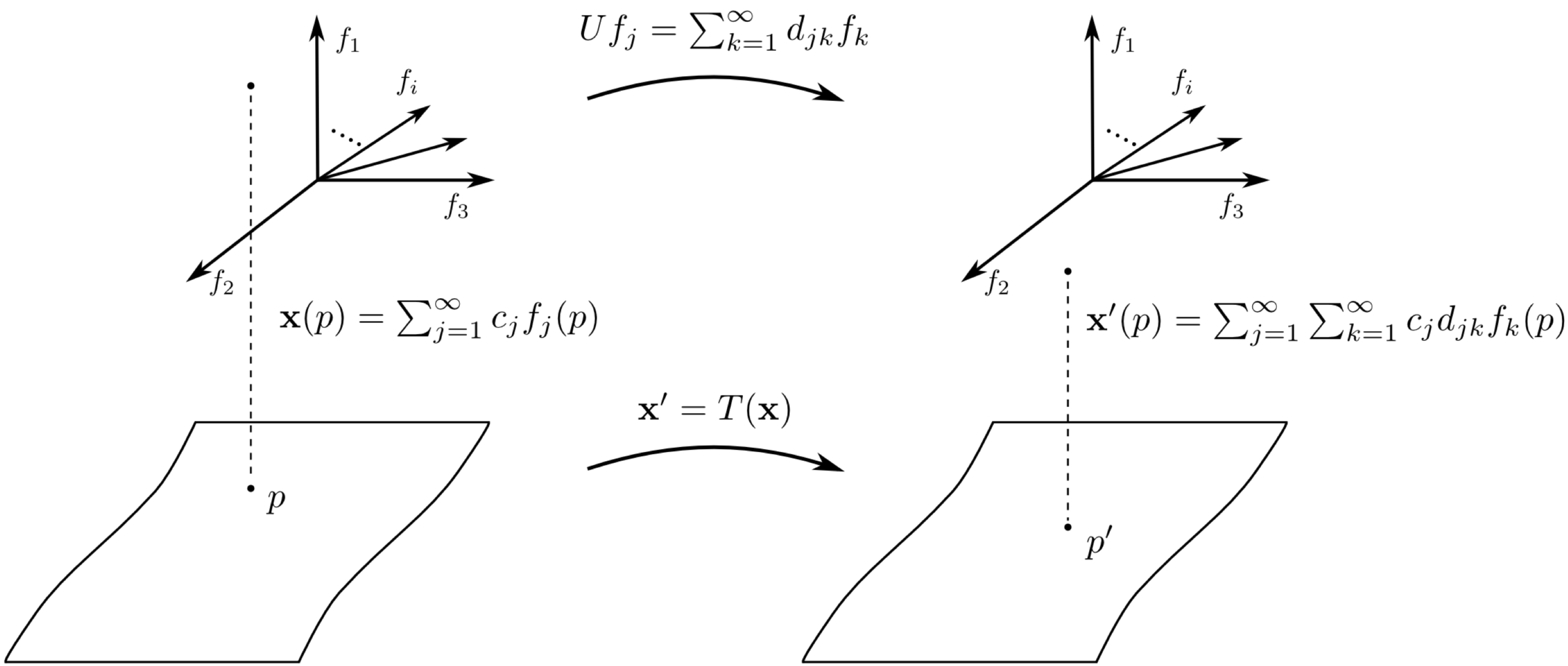
Omri Azencot[1] and Mirela Ben-Chen[1] and Frédéric Chazal[2] and Maks Ovsjanikov[3]

[1]Technion - Israel Institute of Technology
[2] Geometrica, INRIA
[3]LIX, École Polytechnique

New applications

Return to the roots

Introduction



$$\mathbf{x}'(p) = \mathbf{x}(T(p)) = T(\mathbf{x}(p))$$

Operator theory: history and setup

Observables on phase space M $f : M \to \mathbb{C}$

Koopman operator:

$$Uf(x) = f \circ T(x); \quad T : M \to M;$$
$$U^t f(x) = f(S^t x); \quad S^t : M \to M \text{ for every } t \in \mathbb{R}$$

B.O. Koopman "Hamiltonian Systems and Transformations in Hilbert Space", PNAS (1931)
Cf. Carleman (1931), Koopman-vonNeumann (1932)

Vector field case:

$$\dot{\mathbf{x}} = \mathbf{F}(\mathbf{x})$$

Generator equation

$$\frac{\partial f(\mathbf{x},t)}{\partial t} = \mathbf{F}(\mathbf{x}) \cdot \nabla f(\mathbf{x},t).$$

Eigenfunction equation

$$\mathbf{F}(\mathbf{x}) \cdot \nabla \phi(\mathbf{x}) = \lambda \phi(\mathbf{x})$$
$$U^t \phi(\mathbf{x}) = e^{\lambda t} \phi(\mathbf{x})$$

Example:

$$\dot{x} = \{x, H\} \Rightarrow \dot{H} = 0,$$

The Hamiltonian is an eigenfunction of the Koopman operator at eigenvalue 0.

Algebraic Properties of Eigenfunctions

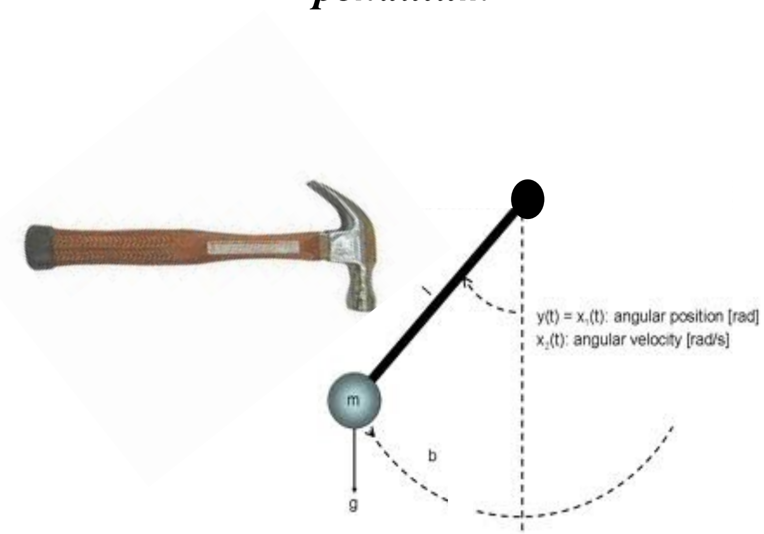
Proposition Let U^t be the Koopman operator family evolving observables on the state space M. Assume $\mathcal{F}$ is a subset of all $\mathbb{C}$-valued functions on a set M that

1. Forms a vector space which is closed under pointwise products of functions, and
2. Contains the constant function whose value is equal to 1.

Then, the set of eigenfunctions forms an Abelian monoid under pointwise products of functions (i.e. $\mathcal{F}$ has identity, associativity, closedness and commutativity). In particular, if $\phi_1, \phi_2 \in \mathcal{F}$ are eigenfunctions of U with eigenvalues β_1 and β_2, then $\phi_1\phi_2$ is an eigenfunction of U with eigenvalue $\beta_1 + \beta_2$.

Invariants and eigenspace at 1

Kicked planar pendulum



$$
\begin{aligned}
x' &= x + y + \varepsilon \sin(2\pi x) \quad [mod\ 1] \\
y' &= y + \varepsilon \sin(2\pi x) \quad [mod\ 1]
\end{aligned}
$$

$\epsilon = 0$

$\epsilon = 0.09$

$\epsilon = 0.18$

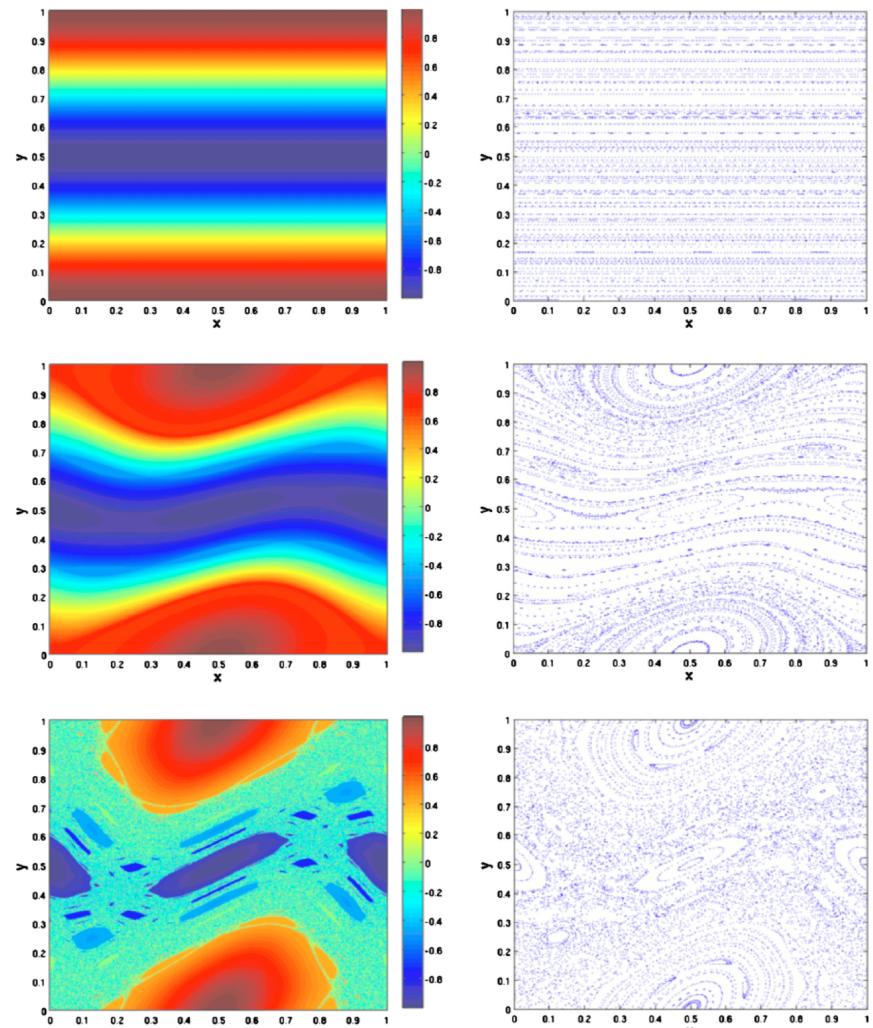


FIG. 1. (Color online) Single-function plots of time averages for the standard map equation (7) (left) and the corresponding phase space portraits (right) done as 100 iterations of 11×11 random trajectories picked from $[0,1]^2$ for the function $f=\cos(2\pi y)$. Top row: $\varepsilon=0$, middle: $\varepsilon=0.09$, bottom: $\varepsilon=0.18$. The grid of 800×800 initial points was used, and the dynamics was run for $t_{final}=30\ 000$ iterations.

The eigenspace at 1 of the Koopman operator contains all L^2 invariants...

There are many!

Left: time averages=eigenfunctions at 1.
Right: state-space (phase space).

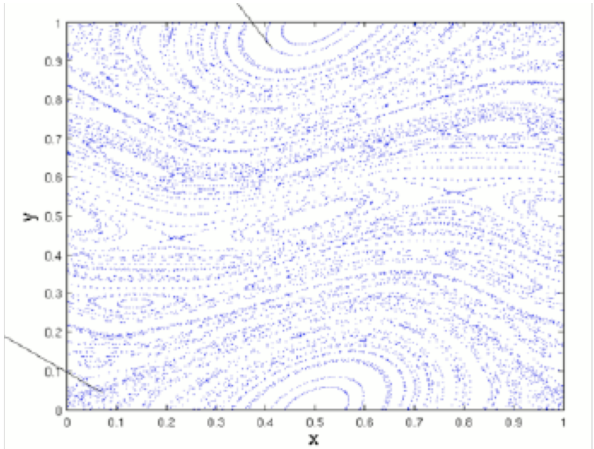
Invariants and the ergodic partition

Theorem 1 *Let M be a compact metric space and $T : M \to M$ a $C^r, r \geqslant 1$, diffeomorphism . Assume there exist a complete system of functions $\{f_i\}, f_i \in C(M)$, i.e. finite linear combinations of f_i are dense in $C(M)$. The ergodic partition of a $C^r, r \geqslant 1$ diffeomorphism $T : M \to M$ on M is*

$$\zeta_e = \bigvee_{i \in \mathbb{N}} \zeta_{f_i}.$$

$$\xi_{f_i} \vee \xi_{f_j} = \{B \in \mathcal{B} | B = C_a \cap C_b, C_a \in \xi_{f_i}, C_b \in \xi_{f_j}\}$$

$$\begin{aligned} x' &= x + y + \varepsilon \sin(2\pi x) \quad [mod\ 1] \\ y' &= y + \varepsilon \sin(2\pi x) \quad [mod\ 1] \end{aligned}$$

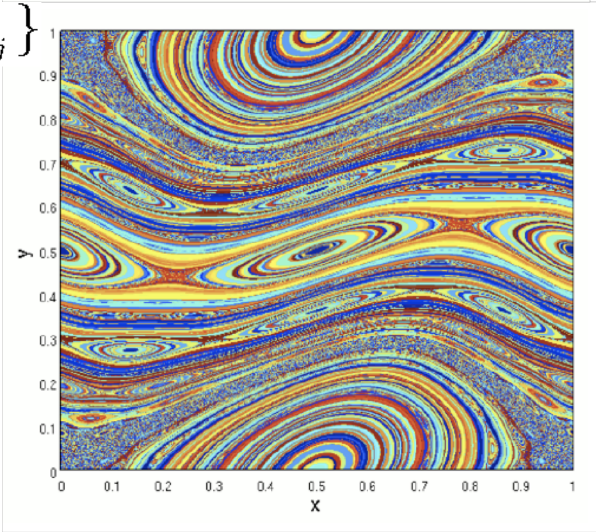


$f_1 = \cos(2\pi y)$

$f_2 = \cos(2\pi x)\cos(2\pi y)$

$f_3 = \sin(4\pi x)\sin(4\pi y)$

$f_4 = \sin(10\pi x)\sin(10\pi y)$



Why is the Hamiltonian special?

Theorem 1 *Let* $\mathbf{v}(\mathbf{x}), \mathbf{x} \in M$ *be a smooth vector field on a two-dimensional manifold* M*, preserving an invariant measure* $\rho | \rho(\mathbf{x}) > 0$*. Then there exists a (unique) smooth eigenfunction* H *of the Koopman operator that in local coordinates* q, p *satisfies*

$$\begin{aligned} \dot{q} &= \frac{\partial H(q,p)}{\partial p}, \\ \dot{p} &= -\frac{\partial H(q,p)}{\partial q}. \end{aligned}$$

where $\dot{()} = d/ds()$*, and* $ds = \rho dt$*.*

Remark 1 *Everything can be ported to coordinate-free setting with few assumptions on the underlying space. E.g. compact contractible manifold will do.*

Why is the Hamiltonian special?

Proof:

1) (from Koopman generator) The equation for an invariant (eigenfunction at 0) G satisfies

$$\dot{q}\frac{\partial G}{\partial q} + \dot{p}\frac{\partial G}{\partial p} = 0, \tag{1}$$

which is satisfied if and only if

$$\dot{q} = f(q,p)\frac{\partial G}{\partial p}, \tag{2}$$

$$\dot{p} = -f(q,p)\frac{\partial G}{\partial q}. \tag{3}$$

where $f(p,q)$ is a smooth function.

The "only if" part comes from geometrical consideration: the vector $(\dot{q},\dot{p})$ is perpendicular to the normal to the surface $G(q,p) = c$ at every point, and thus

$$(\dot{q},\dot{p}) = f(q,p)(\frac{\partial G}{\partial p}, -\frac{\partial G}{\partial q}). \tag{4}$$

Why is the Hamiltonian special?

Proof:

2) (from Perron-Frobenius generator) Now we assume that the system has an invariant measure μ characterized by a smooth density ρ such that $d\mu = \rho dq \wedge dp$. The equation that assures the preservation of μ reads

$$\frac{\partial(\dot{q}\rho)}{\partial q} + \frac{\partial(\dot{p}\rho)}{\partial p} = 0.$$

and thus

$$\frac{\partial(f\frac{\partial G}{\partial p}\rho)}{\partial q} - \frac{\partial(f\frac{\partial G}{\partial q}\rho)}{\partial p} = 0.$$

The above is also the equation for eigenfunction ρ at eigenvalue 0 of the Perron-Frobenius evolution P^t.

Now, if ρ is an eigenfunction of the Perron-Frobenius evolution, we get

$$\frac{\partial(f\rho\frac{\partial G}{\partial p})}{\partial q} - \frac{\partial(f\rho\frac{\partial G}{\partial q})}{\partial p} = \frac{\partial f\rho}{\partial q}\frac{\partial G}{\partial p} - \frac{\partial f\rho}{\partial p}\frac{\partial G}{\partial q} = 0.$$

This implies $f\rho$ is also an invariant of the evolution, i.e., a function of G, $f\rho = F(G)$, leading to

$$\dot{q} = \frac{F(G)}{\rho}\frac{\partial G}{\partial p}, \quad (1)$$

$$\dot{p} = -\frac{F(G)}{\rho}\frac{\partial G}{\partial q}. \quad (2)$$

Why is the Hamiltonian special?

Proof:

3) (from rescaling of time) This implies that there is a function $H(G)$ with $dH/dG = F(G)$ such that

$$\dot{q} = \frac{1}{\rho}\frac{\partial H}{\partial p}, \tag{1}$$

$$\dot{p} = -\frac{1}{\rho}\frac{\partial H}{\partial q}. \tag{2}$$

and thus the underlying system is Hamiltonian, with the Hamiltonian function G. Note that $\rho = 1$ leads to the canonical Hamiltonian structure, but so does the change of time variable $ds = \rho dt$.

- Classically, the existence of the hamiltonian H is proven using the structure of Newtonian dynamics.
- Remarkably, the structure of the dynamics encoded in canonical Hamiltonian equations is *forced* is here derived by pure search for an "equilibrium" measure ρ and an invariant, G.
- In other words, the assumptions on the Koopman and Perron-Frobenius operator spectra - namely that there exists a non-trivial smooth invariant observable, and a strictly positive smooth invariant measure are enough to guarantee the Hamiltonian form of the equations of motion.

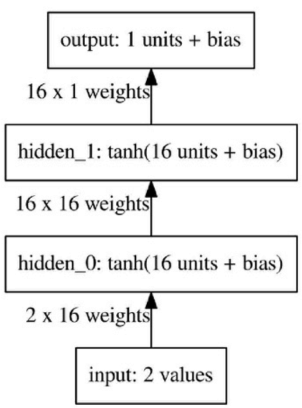
UC SANTA BARBARA

Pendulum Hamiltonian via ANN

Kevrekidis et al:

Approximating H with ANNs

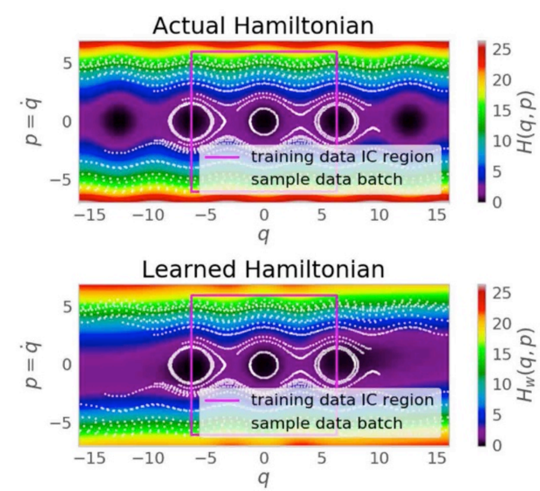
- A similar approximation of H (given only its derivatives) can be done with an Artificial Neural Network (and its automatically constructed derivative)
- The input to the network are the coordinates (q,p), the output is H(q,p)
- To train the network, we use the data $D = \{(q, p, \dot{q}, \dot{p})_k\}$ and the loss function f



$$f(w; q, p, \dot{q}, \dot{p}) = \sum_{k=1}^{4} \lambda_k f_k$$

$$f_1 = \left(\frac{\partial H_w}{\partial p} - \dot{q}\right)^2 \qquad f_2 = \left(\frac{\partial H_w}{\partial q} + \dot{p}\right)^2$$

$$f_3 = (H_w(q_0, p_0) - H_0)^2 \quad f_4 = \left(\frac{\partial H_w}{\partial q}\dot{q} + \frac{\partial H_w}{\partial p}\dot{p}\right)^2 = (\dot{H}_w)^2.$$



Spectral Expansion for Composition Operators

$$
\begin{aligned}
\dot{\mathbf{x}} &= F(\mathbf{x}), \quad \mathbf{x} \in M, && (1)\\
F : M &\to \mathbb{R}^n, && (2)\\
\mathbf{g} : I \times M &\to \mathbb{R}^m, \mathbf{z} \in I && (3)\\
\mathbf{g}_j \in L^2(M), \quad & \forall \quad j \in \{0, ..., n\} && (4)
\end{aligned}
$$

$$
\begin{aligned}
U^t \mathbf{g}(\mathbf{z},\mathbf{x}) &= U^t_s \mathbf{g}(\mathbf{z},\mathbf{x}) + U^t_r \mathbf{g}(\mathbf{z},\mathbf{x})\\
&= \mathbf{g}^*(\mathbf{z}) + \sum_{j=1}^{k} \exp(\lambda_j t)\phi_j(\mathbf{x}) \int_M \mathbf{g}(\mathbf{z},\mathbf{x})\bar{\phi}_j(\mathbf{x})d\mu(\mathbf{x})\\
&+ \int_{-\infty}^{\infty} \exp(i2\pi\alpha t)dE(\alpha)\mathbf{g}(\mathbf{z},\mathbf{x})\\
&= \mathbf{g}^*(\mathbf{z}) + \sum_{j=1}^{k} \exp(\lambda_j t)\phi_j(\mathbf{x})\mathbf{s}_j(\mathbf{z}) + \int_{-\infty}^{\infty} \exp(i2\pi\alpha t)dE(\alpha)(\mathbf{g}(\mathbf{z},\mathbf{x})),
\end{aligned}
$$

I.M. Nonlinear Dynamics, 2005

Heisenberg's Theory as Koopman Theory

Received July 29, 1925

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QUANTUM-THEORETICAL RE-INTERPRETATION OF KINEMATIC AND MECHANICAL RELATIONS

W. HEISENBERG

Position x:

$$x(n, t) = \sum_{-\infty}^{+\infty}{}_{\alpha}\, \mathfrak{A}_{\alpha}(n)\, e^{i\omega(n)\alpha t}$$

$$x(n, t) = \int_{-\infty}^{+\infty} \mathfrak{A}_{\alpha}(n)\, e^{i\omega(n)\alpha t} d\alpha.$$

Classical x^2

$$\mathfrak{B}_{\beta}(n)\, e^{i\omega(n)\beta t} = \sum_{-\infty}^{+\infty}{}_{\alpha}\, \mathfrak{A}_{\alpha}\mathfrak{A}_{\beta-\alpha}\, e^{i\omega(n)(\alpha+\beta-\alpha)t}$$

or

$$= \int_{-\infty}^{+\infty} \mathfrak{A}_{\alpha}\mathfrak{A}_{\beta-\alpha}\, e^{i\omega(n)(\alpha+\beta-\alpha)t} d\alpha,$$

Quantum x^2

$$\mathfrak{B}(n, n-\beta)\, e^{i\omega(n, n-\beta)t} = \sum_{-\infty}^{+\infty}{}_{\alpha}\, \mathfrak{A}(n, n-\alpha)\mathfrak{A}(n-\alpha, n-\beta)\, e^{i\omega(n, n-\beta)t}$$

or

$$= \int_{-\infty}^{+\infty} \mathfrak{A}(n, n-\alpha)\mathfrak{A}(n-\alpha, n-\beta)\, e^{i\omega(n, n-\beta)t} d\alpha,$$

Heisenberg's Theory as Koopman Theory

Namely, Heisenberg observed that one can expand position of a non-harmonic oscillator as

$$x(t) = \sum_{n\in\mathbb{Z}} x_n e^{i\omega_n t}, \ \omega_n = n\omega, \tag{1}$$

where $\omega = dH/dI$. Asking to represent $x^2(t)$ using this expression, we obtain

$$x^2(t) = \sum_{m\in\mathbb{Z}} x_{n-m}x_m e^{i\omega_n t}, \ \omega_n = n\omega,$$

and this did not coincide with experimental observations that suggested dynamic frequencies ω_{nm} that combine as

$$\omega_{nm} = \omega_{nk} + \omega_{km}.$$

This led Heisenberg to conclude that, for a quantum system, one can represent position (or for that matter, any other observable) $\hat{x}(t)$ as

$$\hat{x}(t) = \sum_{n,m\in\mathbb{Z}} x_{nm} e^{i\omega_{nm} t} \tag{2}$$

and thus

$$\hat{x}^2(t) = \sum_{n,m\in\mathbb{Z}} \left(\sum_{k\in\mathbb{Z}} x_{nk}x_{km} \right) e^{i\omega_{nm} t}.$$

Heisenberg's Theory as Koopman Theory

$$\dot{\hat{x}} = \sum_{n,m\in\mathbb{Z}} i\omega_{nm}x_{nm}e^{i\omega_{nm}t}. \qquad (1)$$

In other words,

$$\dot{x}_{nm} = i\omega_{nm}x_{nm}. \qquad (2)$$

The quantum frequencies ω_{nm} were observed to satisfy

$$\omega_{nm} = \frac{1}{\hbar}(E_n - E_m), \qquad (3)$$

for some set of quantities E_k (physically, energies of the system).

Let $x_{nm}(t) = x_{nm}e^{i\omega_{nm}t}$. We get

$$\dot{x}_{nm}(t) = i\frac{1}{\hbar}(E_n - E_m)x_{nm}(t), \qquad (4)$$

and, defining the matrix $\hat{x}$ by $\hat{x}_{mn} = x_{nm}(t)$ to obtain

$$i\hbar\dot{\hat{x}} = [\hat{x}, \hat{E}], \qquad (5)$$

where $\hat{E} = E_n\delta_{nm}$ is a diagonal matrix with energies E_k on the diagonal, and $[A, B] = AB - BA$ for matrices A and B.

Postulate using correspondence principle:

$$\hat{E} = \hat{p}^2/2 + V(\hat{x}). \qquad (6)$$

Noting that a new variable $\hat{p}$ (the quantum analogue of momentum) entered in the energy relationship, we can derive, analogously

$$i\hbar\dot{\hat{p}} = [\hat{p}, \hat{E}]. \qquad (7)$$

x_{nm} is Koopman operator eigenfunction!

Heisenberg's Theory as Koopman Theory

It is interesting to note the little known Pauli identity

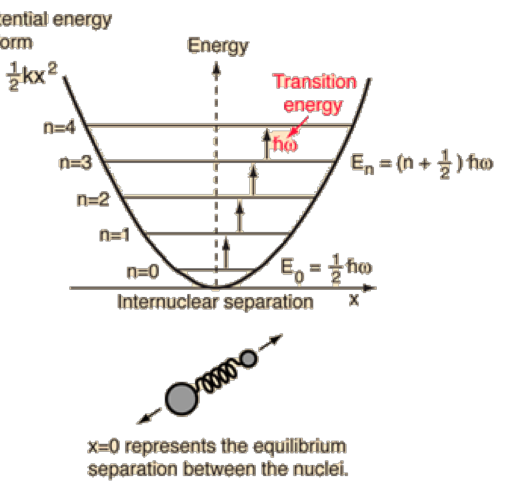
$$x_{nm} = \int_{-\infty}^{\infty} \hat{x}\psi_n(x)\psi_m(x)dx$$

Which implies - using the interpretation of

$$\hat{x} = \sum_{m,n} x_{mn} e^{i\omega_{mn}t}$$

as the Koopman Mode Decomposition - that the Koopman eigenfunctions in quantum mechanics are precisely

$$\phi_{nm} = \psi_n \psi_m.$$



For quantum harmonic oscillator, the energy levels read

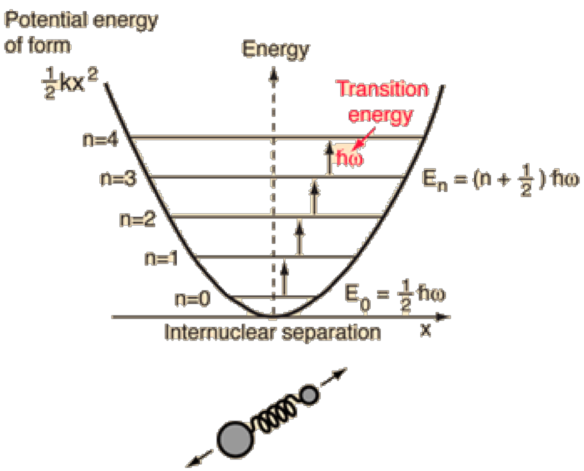
$$E_n = \hbar(\frac{\omega}{2} + n\omega) = \hbar\omega(n + 1/2), \tag{1}$$

and thus, by Bohr's rule, the associated frequencies are

$$\omega_{n,m} = \frac{1}{\hbar}(E_n - E_m) = \omega(n - m). \tag{2}$$

- Consistent with the spectrum of the Koopman operator associated with the classical harmonic oscillator, restricted to orbits with the discrete energy levels.
- Indicates that the harmonic oscillator frequencies are the consequence of a nonlinear observation on the linear underlying harmonic oscillator process.

Dirac's Raising and Lowering Operator



Dirac's creation an annihilation (equivalently, raising and lowering) operators for the harmonic oscillator,

$$\hat{a}_+ = \frac{1}{\sqrt{2hm\omega}}(i\hat{p} + m\omega\hat{q}) \quad (1)$$

$$\hat{a}_- = \frac{1}{\sqrt{2hm\omega}}(i\hat{p} + m\omega\hat{q}) \quad (2)$$

$$(3)$$

are the quantized version of eigenfunctions of the classical harmonic oscillator of frequency ω associated with Koopman eigenvalues $\pm i\omega$: Let

$$\dot{q} = p/m,$$
$$\dot{p} = -m\omega^2 q. \quad (4)$$

Then

$$\phi_1 = \frac{1}{2}(q + i\frac{p}{m\omega}), \quad (5)$$

and

$$\hat{a}_+ = \frac{m\omega}{\sqrt{2hm\omega}}\hat{\phi}_1 = \sqrt{\frac{m\omega}{2h}}\hat{\phi}_1 \quad (6)$$

where $\hat{\phi}_1$ is the quantized operator

$$\hat{\phi}_1 = \frac{1}{2}(\hat{q} + i\frac{\hat{p}}{m\omega}). \quad (7)$$

In fact, multiplication operators

$$\hat{L}^+ f = \phi_1 f \quad (1)$$
$$\hat{L}^- f = \phi_1^c f \quad (2)$$

are the raising and lowering operators for the Koopman operator of the classical harmonic oscillator (and more generally, multiplication by principal eigenfunctions are ladder operators for classical Koopman operators.

Densities on Observables

Let $M = \mathbb{R}$ and $(x,t) \in R = \mathbb{R} \times \mathbb{R}$. Let v be a smooth vector field on $\mathbb{R}$. The wavefunction ρ (we will call it the true wavefunction or TW) satisfies

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho v}{\partial x} = 0, \tag{1}$$

Let the observable $f : \mathbb{R} \to \mathbb{C}$ be defined by

$$f = e^{-iY}, \tag{2}$$

where $Y(x,t)$ is smooth (at least in C^2). This implies that the observable wavefunction (OW) ψ defined by

$$\psi = \frac{\rho}{i\frac{\partial Y}{\partial x} e^{iY}}. \tag{3}$$

is the density of a complex measure of the observable $f = e^{-iY}$ corresponding with the TW ρ, since

$$\frac{df}{dx} = i\frac{\partial Y}{\partial x} e^{iY}. \tag{4}$$

Densities on Observables: A Schrodinger-Like Formalism

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A Dirac-Like Equation

After some calculation, we get

$$\psi_t = -v\psi_x + \psi\left(-v_x - \frac{v}{Y_x}Y_{xx} - \frac{Y_{xt}}{Y_x} - i(Y_t + vY_x)\right)$$

This is the Dirac-like equation that governs the observable wavefunction evolution.

If the observable is real, with $Y = iK$, we get

$$\psi_t = -v\psi_x + \psi\left(-v_x + K_t - \frac{v}{K_x}(K_{xx} - K_x^2) - \frac{K_{xt}}{K_x}\right).$$

Conclusions

- Discovery of the fundamental laws of classical physics (e.g. existence of differential equations in Hamiltonian form) is enabled by assumptions on the eigenspace at 0 of the Koopman and Perron-Frobenius operators.
- Heisenberg's discovery of quantum mechanics can be couched in the Koopman Mode Decomposition language. This leads to the conclusion that Quantum Dynamics is not linear.
- Spectrum of the quantum Harmonic Oscillator is consistent with the spectrum of the Koopman operator of the classical Harmonic Oscillator.
- Dirac's raising and lowering operators can be motivated by their classical versions
- Equation for a wavefunction of an observable on a dynamical system yields a Dirac-Schrodinger type equation.

Conclusions

This indicates the wave function in quantum mechanics represents "knowledge"

Wilczek in his online note *Notes on Koopman von Neumann Mechanics, and a Step Beyond*' says

"In the classical theory, at least, it seems hard to avoid the implication that the wave function re ects our knowledge of the system. More generally, it seems that controversies over the interpretation of quantum theory can be illuminated by comparing with this parallel formulation of classical physics."