Notes on Koopman von Neumann Mechanics, and a Step Beyond

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1. Classical mechanics, as usually formulated, seems to inhabit a different conceptual universe from quantum mechanics. Koopman and von Neumann developed a mathematical formulation of classical mechanics using concepts usually associated with quantum theory. In this formulation we have wave functions, Hilbert spaces, operators, ... The Koopman-von Neumann (KvN) formulation has proved useful as a technical device in several applications, notably in ergodic theory. It deserves to be better known among physicists, because it gives a new perspective on the conceptual foundations of quantum theory, and it may suggest new kinds of approximations and even new kinds of theories (which is what we'll be heading toward).

2. Let us recall the phase space formulation of distributions in classical mechanics, as is often used in statistical mechanics and kinetic theory. For simplicity in notation I'll write equations for a system with one degree of freedom, but their generalization is straightforward, and when it becomes necessary we'll add in complications without much ado.

The quantity of interest is the density $\rho(x, p, t)$. It is a non-negative real quantity, to be interpreted as the probability that we'll find a particle with momentum p at point x at time t, using the measure $\int dx\, dp$. Liouville's theorem in mechanics tells us that the flow of this fluid is incompressible. So we have

$$0 \;=\; \frac{d\rho}{dt} \;=\; \frac{\partial \rho}{\partial t} + \dot{x}\frac{\partial \rho}{\partial x} + \dot{p}\frac{\partial \rho}{\partial p} \tag{1}$$

or

$$\begin{aligned} \frac{\partial \rho}{\partial t} &= -\,\dot{x}\frac{\partial \rho}{\partial x} - \dot{p}\frac{\partial \rho}{\partial p} \\ &= -\,\frac{\partial H}{\partial p}\,\frac{\partial \rho}{\partial x} + \frac{\partial H}{\partial p}\,\frac{\partial \rho}{\partial p} \end{aligned} \tag{2}$$

which serves as a dynamical equation for ρ. If we multiply both sides by i, we get an equation having a family resemblance to the Schrödinger equation.

3. With that motivation, we introduce a complex wave function $\psi(x, p)$ which obeys that equation:

$$\begin{aligned} i\frac{\partial \psi}{\partial t} &= i(-\frac{\partial H}{\partial p}\frac{\partial \psi}{\partial x} + \frac{\partial H}{\partial p}\frac{\partial \psi}{\partial p}) \\ &\equiv \hat{L}\psi \end{aligned} \tag{3}$$

where the last line defines the Liouville operator $\hat{L}$.

A first simple but profound point is that $\rho_\psi \equiv |\psi(x,p)|^2$ then satisfies Eqn. (1). Thus, when interpreted as a probability density, it satisfies the appropriate dynamical equation. This result follows immediately by application of the Leibniz rule for derivatives of products.

A second is that $\hat{L}$ is an Hermitian operator with respect to the inner product

$$\langle \psi|\psi \rangle \;=\; \int dx\, dp\, \psi^*(x,p)\psi(x,p) \tag{4}$$

One proves this through an integration by parts. Note that the i is important here, which is the reason it was introduced. The equality of mixed derivatives, $\frac{\partial^2 H}{\partial p \partial x} = \frac{\partial^2 H}{\partial x \partial p}$ also comes in, canceling the terms that arise from the functional factors in $\hat{L}$.

4. Now we want to build up the formalism along lines parallel to the conventional treatment of quantum theory, introducing operators and observables. In fact we will use the same axioms for both classical and quantum theory, except that in the classical theory the operators for position and momentum commute, while in the quantum theory they do not

$$[\hat{x}, \hat{p}] \;=\; 0 \qquad \text{(classical)} \tag{5}$$

$$[\hat{x}, \hat{p}] \;=\; i\hbar \qquad \text{(quantum)} \tag{6}$$

We will not *assume* the functional form of the wave function, but derive it – with different results, in the two cases – as a possible realization of the fundamental Hilbert space structure, starting from more abstract principles.

An appropriate set of axioms includes the following

1. Normalization: The wave function for an individual system satisfies

$$\langle \Psi(t)|\Psi(t)\rangle \;=\; 1 \tag{7}$$

2. Observables: Observables are defined by Hermitian operators. The expectation value of an observable $\hat{A}$ at time t is given by

$$\overline{A(t)} \;=\; \langle\Psi(t)|\hat{A}|\Psi(t)\rangle \tag{8}$$

3. Born rule: The probability of measuring the value a of an observable $\hat{A}$ at time t is given by

$$\mathrm{Pr(a)} \;=\; |\,\Pi_a|\Psi(t)\rangle\,|^2 \tag{9}$$

   where Π_a is the projection operator onto the eigenspace of $\hat{A}$ with eigenvalue a.

4. Composite Systems: Composite systems are described by tensor product Hilbert spaces.

We will not be developing a rigorous axiomatic approach here; I'm recalling this material just to set the context. (Dirac's book is a great and inspiring development of quantum mechanics along these lines.)

Those are general "kinematic" axioms. To implement a particular dynamics, we must specify further structure.

The operators $U(t)$ that connect wave functions at time 0 to wave functions at time t,

$$|\Psi(t)\rangle \;=\; U(t)|\Psi(0)\rangle \tag{10}$$

give us a unitary representation of the group of time translations. According to Stone's theorem, there must be a generating Hermitean operator, with

$$i\frac{d|\Psi\rangle}{dt} \;=\; \hat{L}|\Psi\rangle \tag{11}$$

In conventional quantum theory $\hat{L}$ is the operator Hamiltonian, but in the classical theory it will be a related yet different operator, as we shall see.

5. Here we will consider Newtonian mechanics, and implement the correspondence principle by demanding Newton's equations for the expectation values of observables for position and momentum, in the form

$$\begin{aligned}\frac{d}{dt}\langle\hat{x}\rangle &= \langle\hat{p}/m\rangle\\ \frac{d}{dt}\langle\hat{p}\rangle &= \langle-\widehat{U'(x)}\rangle\end{aligned} \tag{12}$$

Using Eqn. (11) and the axioms, we can spell out the first of these equations as

$$\begin{aligned}\frac{d}{dt}\langle\Psi(t)|\hat{x}|\Psi(t)\rangle &= (\frac{d}{dt}\langle\Psi(t)|)\hat{x}|\Psi(t)\rangle + \langle\Psi(t)|\hat{x}\frac{d}{dt}|\Psi(t)\rangle \\ &= i\langle\Psi(t)|[\hat{L},\hat{x}]|\Psi(t)\rangle \\ &= \langle\Psi(t)|\frac{\hat{p}}{m}|\Psi(t)\rangle \qquad (13)\end{aligned}$$

Since this is to hold for any wave function, we have the operator equation

$$i[\hat{L},\hat{x}] = \frac{\hat{p}}{m} \qquad (14)$$

Similarly, we have

$$i[\hat{L},\hat{p}] = -\widehat{U'(x)} \qquad (15)$$

Here the hat $(\widehat{\ })$ notation which indicates operators is used to indicate that we take the derivative of the potential with x treated as a number, and then convert to operators at the end. This notation will be very useful to us.

6. Now if we have the classical (trivial) commutation relation $[\hat{x},\hat{p}]=0$, then we cannot construct an $\hat{L}$ that implements Eqns. (14, 15) out of the dynamical variables $\hat{x},\hat{p}$ alone. Stone's theorem tells us there is such an operator, but it does not guarantee that it can be expressed in terms of some given set of operators.

To remedy the situation, we introduce two additional Hermitian operators $\widehat{\lambda_x},\widehat{\lambda_p}$ which satisfy

$$[\hat{x},\widehat{\lambda_x}] = i \qquad (16)$$

$$[\hat{p},\widehat{\lambda_p}] = i \qquad (17)$$

with all other commutators involving these variables vanishing. (Soon we shall construct these operators explicitly.) With the help of these additional operators, we can construct a satisfactory $\hat{L}$, which implements the correspondence principle dynamics, as

$$\hat{L} = \frac{\hat{p}}{m}\widehat{\lambda_x} - \widehat{U'(x)}\widehat{\lambda_p} \qquad (18)$$

7. Now we use a particular choice of basis to bring the results into a more familiar, intuitively accessible form. Since $\hat{x}$, $\hat{p}$ are commute, and (we

can assume) form a complete set of commuting observables, we form a basis of simultaneous eigenstates, according to

$$\begin{aligned} \hat{x}|x,p\rangle &= x|x,p\rangle \\ \hat{p}|x,p\rangle &= p|x,p\rangle \end{aligned} \tag{19}$$

with the normalization condition

$$\langle x'',p''|x',p'\rangle = \delta(x''-x')\delta(p''-p') \tag{20}$$

From

$$[\hat{x},\widehat{\lambda_x}] = i \tag{21}$$

we easily derive

$$[\hat{x}^n,\widehat{\lambda_x}] = in\hat{x}^{n-1} \tag{22}$$

and using Taylor's series

$$[\widehat{f(x)},\widehat{\lambda_x}] = i\widehat{f'(x)} \tag{23}$$

We can represent wave functions in the form

$$\langle x,p|\Psi(t)\rangle = \psi(x,p,t) \tag{24}$$

and then we have

$$\widehat{\lambda_x} \sim -i\frac{\partial}{\partial\hat{x}} \rightarrow -i\frac{\partial}{\partial x} \tag{25}$$

in this representation. Similarly,

$$\widehat{\lambda_p} \rightarrow -i\frac{\partial}{\partial p} \tag{26}$$

The Schrödinger equation, in this representation, becomes the wave equation

$$i\frac{\partial\psi}{\partial t} = \Big(\frac{p}{m}(-i\frac{\partial}{\partial x}) - U'(x)(-i\frac{\partial}{\partial p})\Big)\psi \tag{27}$$

– which brings us, of course, back to our motivational starting point.

8. For an observable $\widehat{A(x,p)}$ constructed from $\hat{x},\hat{p}$, we have for the expected value at time t

$$\begin{aligned} \langle\Psi(t)|\widehat{A(x,p)}|\Psi(t)\rangle &= \int dx\,dp\,\psi^*(x,p,t)A(x,p)\psi(x,p,t) \\ &= \int dx\,dp\,A(x,p)\rho(x,p,t) \end{aligned} \tag{28}$$

as it should be, realizing the interpretation of $\psi^*\psi$ as a probability distribution in phase space.

We can, however, also consider other sorts of observables – that is, Hermitian operators – involving $\widehat{\lambda_x}, \widehat{\lambda_p}$ as well as $\hat{x}, \hat{p}$. These do not have a direct classical meaning. Indeed, in going from the classically meaningful $\rho(x,p)$ to the "square root" $\psi(x,p)$ there is an arbitrary, position (in phase space) dependent phase choice – a sort of gauge transformation. Only observables which do not depend on that phase choice will be meaningful, classically. In other words, the classical content of the theory is restricted to gauge invariant observables.

Nevertheless the non-classical observables are perfectly well defined operators in Hilbert space. They are realized as differential operators, as we've seen. They will play an important role in the generalized, mixed quantum/classical theories we introduce below.

We should also note that as it stands the new gauge symmetry is not dynamical, nor does it allow time-dependent gauge transformations. It may be interesting to lift those restrictions, but I will not discuss that possibility further here.

9. It is worth a short digression to make contact with traditional Newtonian point particle mechanics. This is most naturally done through the method of characteristics, as follows. A first-order partial differential equation

$$f^j(y^k)\partial_j G(y^k) \;=\; 0 \tag{29}$$

we note that G will be constant along the solution curves of the system of ordinary differential equations

$$\frac{dy^k}{d\lambda} \;=\; f^k \tag{30}$$

Thus we can solve the partial differential equation, given the initial data on a codimension one hypersurface, by drawing the characteristics through it, and transporting the data.

In our context, the characteristics of

$$\frac{\partial\psi}{\partial t} + \frac{p}{m}\frac{\partial\psi}{\partial x} - U'(x)\frac{\partial\psi}{\partial p} \;=\; 0 \tag{31}$$

are the solutions of

$$\frac{dt}{d\lambda} \;=\; 1$$

$$\begin{aligned}\frac{dx}{d\lambda} &= \frac{p}{m} \\ \frac{dp}{d\lambda} &= -U'(x)\end{aligned} \tag{32}$$

– in other words, the Newtonian trajectories. Thus delta-function solutions, with definite initial values of x, p, will follow the Newtonian equations for a point particle.

10. It is pleasant that the basic object in the Koopman-von Neumann framework, that is the wave function, lives in a complex vector space. Thus we have the usual notion of linear superposition. That superposition principle is not available for ρ, which is constrained to be real and non-negative.

11. Conventional quantum mechanics can be developed axiomatically along similar lines, but the nontrivial commutator $[\hat{x}, \hat{p}] = i$ leads to two major qualitative differences.

1. Now we can implement Eqns. (14, 15) using only the dynamical variables $\hat{x}, \hat{p}$. Indeed, we find

   $$\hat{L} = \frac{\hat{p}^2}{2m} + \widehat{U(x)} = \hat{H} \tag{33}$$

   – the familiar result that the Hamiltonian operator generates temporal evolution.

2. Now $\hat{x}$ (or $\hat{p}$) by itself forms a complete set of commuting observables. Accordingly, we can use a basis of eigenstates $|x\rangle$ with

   $$\begin{aligned}\hat{x}|x\rangle &= x|x\rangle \\ \langle x''|x'\rangle &= \delta(x'' - x')\end{aligned} \tag{34}$$

   and represent wave functions using

   $$\langle x|\Psi(t)\rangle = \psi(x,t) \tag{35}$$

12. In the classical theory, as in the quantum theory, a measurement gives us information on the wave function, that amounts to a projection in Hilbert space. In the classical theory, it "collapses the wave function" in the sense that in calculating the subsequent evolution of the classical system, we should take into account the information we've acquired, and

calculate relative probabilities that incorporate that knowledge, using an appropriate (collapsed) wave function. In the classical theory, at least, it seems hard to avoid the implication that the wave function reflects 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.

13. We obtain an interesting perspective on the classical theory by renaming the variables, as follows:

$$\begin{aligned} \hat{x} &\rightarrow \widehat{x_1} \\ \hat{p} &\rightarrow \widehat{p_2} \\ \widehat{\lambda_x} &\rightarrow \widehat{p_1} \\ \widehat{\lambda_p} &\rightarrow -\widehat{x_2} \end{aligned} \tag{36}$$

After this renaming, we find that our dynamical variables obey the conventional (Heisenberg) quantum commutation relations for two particle degrees of freedom.

$\widehat{x_1}, \widehat{p_2}$ form a complete set of commuting observables, so we can form wave functions $\psi(x_1, p_2, t)$ which, according to our preceding work, obey the Schrödinger equation

$$i\frac{\partial\psi}{\partial t} = (\frac{p_2}{m}(-i\partial_{x_1}) - U'(x_1)(i\partial_{p_2}))\psi \tag{37}$$

This looks like a more-or-less normal quantum system, but we know, by construction, that it has a "secret" classical core.

Observables of the form $G(\widehat{x_1}, \widehat{p_2})$ correspond to the observables of the original classical theory. More general observables, involving $\widehat{x_2}, \widehat{p_1}$, are not observables of the original classical theory. Nevertheless, they can be calculated unambiguously from the wave function, by using Fourier transforms.

The generator of temporal evolution, according to Eqn. (37), is the operator

$$\widehat{H_{\text{temporal}}} = \frac{\widehat{p_2}}{m}\widehat{p_1} + \widehat{U'(x_1)}\widehat{x_2} \tag{38}$$

This is quite different from the operator form of the classical Hamiltonian, i.e.

$$\widehat{H_{\text{C}}} = \frac{\widehat{p_2}^2}{2m} + U(\widehat{x_1}) \tag{39}$$

One might therefore worry about conservation laws, boundedness of energy, and so forth. It is therefore important to observe that for $\widehat{x_1}, \widehat{p_2}$, and therefore for all *classical* observables $\widehat{A(x_1, p_2)}$, one has the relation

$$[\widehat{H_{\text{temporal}}}, \hat{A}] \;=\; i(-\widehat{\frac{\partial H_{\text{C}}}{\partial p_2}\frac{\partial A}{\partial x_1} + \frac{\partial H_{\text{C}}}{\partial x_1}\frac{\partial A}{\partial p_2}}) \tag{40}$$

which – for classical observables – links commutators of the temporal evolution operator of the quantum system with the Poisson bracket of the classical system. Thus the classical conservation laws remain valid, with the conserved quantities taking their usual form. $\widehat{H_{\text{temporal}}}$ is of course also a conserved quantity, though it is not a *classical* observable.

To round out this discussion, let us note that the classical Lagrangian corresponding to the temporal Hamiltonian is

$$L_{\text{temporal}} \;=\; m\dot{x}_1\dot{x}_2 - U'(x_1)x_2 \tag{41}$$

14. Alternatively, we can do a further renaming

$$\begin{aligned} \widehat{x_2} &\;\to\; \widehat{-p_2} \\ \widehat{p_2} &\;\to\; \widehat{x_2} \end{aligned} \tag{42}$$

This is a canonical transformation, which leaves the commutation relations unchanged.

Now we have $\widehat{x_1}, \widehat{x_2}$ as the complete set of commuting observables, and the basic classical dynamical variables. The temporal Hamiltonian is

$$\widehat{H_{\text{temporal}}} \;=\; \frac{\widehat{x_2}}{m}\widehat{p_1} \;-\; \widehat{U'(x_1)}p_2 \tag{43}$$

and the corresponding Lagrangian vanishes.

15. How is the "determinism" of classical mechanics, as contrasted with quantum mechanics, reflected here? Both theories have a Born rule, which appears probabilistic . Both implement unambiguous time evolution, given an initial value for the wave function, which appears deterministic. The difference is that in the classical theory one can have states – the $|x, p\rangle$ – wherein all the interesting observables variables have definite values. That is not possible in the quantum theory. No matter what state we are in there will always be questions for which the answer is probabilistic, even though the dynamical equations are completely definite.

16. Now let us consider the possibility of constructing new kinds of theories, involving both quantum and classical dynamical variables. We have

$$
\begin{aligned}
[\widehat{x_{\rm Q}}, \widehat{p_{\rm Q}}] &= i \\
[\widehat{x_{\rm C}}, \widehat{p_{\rm C}}] &= 0
\end{aligned}
\tag{44}
$$

We can follow the preceding constructions of the separate theories in a straightforward way, until we reach the following point, when we try to couple them. The correspondence principle suggest both

$$
i[\hat{L}, \widehat{p_{\rm Q}}] \; = \; -\,\partial_{x_{\rm Q}} \widehat{U(x_{\rm Q}}, x_{\rm C}) \tag{45}
$$

and

$$
i[\hat{L}, \widehat{p_{\rm C}}] \; = \; -\,\partial_{x_{\rm C}} \widehat{U(x_{\rm Q}}, x_{\rm C}) \tag{46}
$$

The second of these requires, as we've seen, that we bring in the operator $\widehat{\lambda_{p_{\rm C}}}$. But that operator will then carry infest the left-hand side of Eqn. (45), where it is not wanted.

There are two simple options for dealing with this difficulty.

1. Option 1: We can add $U(\widehat{x_{\rm C}, x_{\rm Q}})$ to $\hat{L}$. Then we satisfy Eqn. (45), but find zero in place of the right-hand side of Eqn. (46). The classical system therefore evolves on its own, independent of the quantum system, which however it does affect. (We can include of course allow non-trivial self-dynamics for the classical theory, as before.) In effect, the classical system acts as an external field imposed on the quantum system.

2. Option 2: We can add $-\partial_{x_{\rm C}} \widehat{U(x_{\rm C}}, x_{\rm Q})\widehat{\lambda_{p_{\rm C}}}$ to $\hat{L}$. This implements Eqn. (46) as it stands, but gives us

$$
i[\hat{L}, \widehat{p_{\rm Q}}] \; = \; -\,\partial_{x_{\rm Q}} \partial_{x_{\rm C}} \widehat{U}(x_{\rm Q}, x_{\rm C}) \widehat{\lambda_{p_{\rm C}}} \tag{47}
$$

in place of Eqn. (45). The evolution of the quantum system now depends on the classical system through its *non-classical* observable $\widehat{\lambda_{p_{\rm C}}}$. That very interaction gives us access to the non-classical observable, and lifts it from being a purely formal construct, which it was within the classical theory, into becoming a physically meaningful quantity. This is a much less familiar, but apparently consistent, way to construct mixed theories.

We can also add both terms. In this way we get both the expected interactions, plus an additional term whereby the classical theory perturbs the quantum theory, through a classically determined but non-classical interaction.

Of course, if we do not insist on deriving our coupling from a classical correspondence principle, we have the option of coupling the classical to the quantum theory in much more general ways.

17. It is natural to consider commutation relations in the form

$$[\hat{x}_j, \hat{p}_k] \ = \ iA_{jk} \tag{48}$$

with a c-number antisymmetric expression A. By linear transformations of the variables, we can put A into a canonical form, with blocks of paired variables satisfying

$$[\hat{x}_j, \hat{p}_k] \ = \ i\delta_{jk} \tag{49}$$

together with some number (invariant under linear transformations) of pairs with zero commutators. From this more abstract perspective, it is quite natural to consider mixed quantum-classical dynamics.

18. One may consider locking of quantum to classical variables, so that the effective low-energy degrees of freedom are a mixture of fundamental degrees of freedom of mixed kinds. An interaction of the form

$$\delta\hat{H} \ = \ \mu^2(\widehat{x_{\rm Q}} - \widehat{x_{\rm C}})^2 \tag{50}$$

encourages such behavior.

19. Dyson has emphasized that severe difficulties arise when one attempts to give direct experimental meaning to quantum effects in gravity. Also, notoriously, straightforward quantization of gravity, in the form of general relativity, apparently leads to ultraviolet divergences. Thus it may be interesting to consider the possibility that characteristically gravitational degrees of freedom are not quantized at all. The theoretical technology developed above can support mathematically consistent exploration of such possibilities.