Operational Dynamic Modeling Transcending Quantum and Classical Mechanics

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We introduce a general and systematic theoretical framework for operational dynamic modeling (ODM) by combining a kinematic description of a model with the evolution of the dynamical average values. The kinematics includes the algebra of the observables and their defined averages. The evolution of the average values is drawn in the form of Ehrenfest-like theorems. We show that ODM is capable of encompassing wide-ranging dynamics from classical non-relativistic mechanics to quantum field theory. The generality of ODM should provide a basis for formulating novel theories.

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Introduction.—One primary goal in science is to construct models possessing predictive capability. This endeavor is usually achieved by trial and error, with a proposed model either subsequently revised or completely discarded if its predictions do not agree with experimental results. Generally such a process is slow; hence, automatization has been attempted [1,2].

In this Letter, we develop a universal and systematic theoretical framework for operational dynamic modeling (ODM) based on the evolution of dynamical average values. As an illustration of ODM's scope, we infer quantum, classical, and unified quantum-classical mechanics. In order to construct a system's dynamical model, we first postulate an associated kinematic description consisting of two independent components: (i) the definition of the observables' average and (ii) the algebra of the observables. ODM applied to observable data, given in the form of Ehrenfest-like theorems [see, e.g., Eq. (1)], returns the dynamical model (see Fig. 1 in the Supplemental Material [3] for a graphical summary). The system's kinematic description can also be deduced from complementary experiments. For example, if the results of a sequential measurement depend on the measurements' order, then the algebra of observables must be noncommutative [see comments after Eqs. (3) and (13)]. Limited access to experiments capable of firmly establishing the kinematics does not preclude hypothesizing plausible kinematic descriptions. Some of these hypotheses may be rejected within ODM by revealing their incompatibility with observable dynamical data [4].

In the spirit of ODM, starting from the Ehrenfest theorems [Eq. (2)], we will obtain the Schrödinger equation if the momentum and coordinate operators obey the canonical commutation relation, and the classical Liouville equation if the momentum and coordinate operators commute. To establish a link between quantum and classical mechanics, we introduce a generalized algebra of observables, incorporating both quantum and classical kinematics, that ultimately leads to a unified quantum-classical mechanics. Most importantly, we will show that ODM is applicable to a wide range of physical models from nonrelativistic classical mechanics to quantum field theories, thus making ODM an important tool for formulating future models.

Preparing dynamical data.—In the current work, we present the conceptual and theoretical framework of ODM, putting aside issues of handling noise-contaminated experimental data. Assume we have multiple copies of either a quantum or classical system (without loss of generality we consider single-particle one-dimensional systems throughout). Suppose we can precisely measure different copies of the particle's coordinate x and momentum p at times $\{t_k\}_{k=1}^K$. Upon performing ideal measurements of the coordinate or momentum on the nth copy, we experimentally obtain $\{x_n(t_k)\}$ and $\{p_n(t_k)\}$, $n = 1, \ldots, N$, requiring a total of $2KN$ observations. Time interpolation of these data points returns the functions $x_n(t)$ and $p_n(t)$. We may then calculate the statistical moments $\overline{[x(t)]^l} = \frac{1}{N}\sum_{n=1}^N [x_n(t)]^l$ and $\overline{[p(t)]^l} = \frac{1}{N}\sum_{n=1}^N [p_n(t)]^l$ for $l = 1, 2, 3, \ldots$ We make the ansatz, resembling a Taylor series with coefficients a_l, b_l, $c_{k,l}$, d_l, e_l, and $f_{k,l}$, that the first derivative of $\overline{x(t)} = \overline{[x(t)]^1}$ and $\overline{p(t)} = \overline{[p(t)]^1}$ satisfy

$$\frac{d}{dt}\overline{x(t)} = \sum_l (a_l \overline{[x(t)]^l} + b_l \overline{[p(t)]^l}) + \sum_{k,l \neq 0} c_{k,l} \overline{[x(t)]^l [p(t)]^k},$$

$$\frac{d}{dt}\overline{p(t)} = \sum_l (d_l \overline{[x(t)]^l} + e_l \overline{[p(t)]^l}) + \sum_{k,l \neq 0} f_{k,l} \overline{[x(t)]^l [p(t)]^k}.$$

For nondissipative quantum and classical systems, these relations reduce to

$$m\frac{d}{dt}\overline{x(t)} = \overline{p(t)}, \qquad \frac{d}{dt}\overline{p(t)} = \overline{-U'(x)}(t), \tag{1}$$

where $\overline{-U'(x)}(t) = \sum_l d_l \overline{[x(t)]^l}$.

Kinematic description.—Generalizing Schwinger's motto "quantum mechanics: symbolism of atomic measurements" [6], we add the adaptation that any physical model is a symbolic representation of the experimental evidence supporting it. The mathematical symbolism for this purpose needs to be considered. A formalism specialized to describe a specific class of behavior (e.g., classical mechanics expressed in terms of phase space trajectories) can be effective, but it may be unsuitable for connecting different classes of phenomena (e.g., unifying quantum and classical mechanics). In this case a general and versatile formalism is preferred. Building a formalism around Hilbert space is a suitable candidate for this role. Hilbert space is well understood, rich in mathematical structure, and convenient for practical computations.

Consider the postulates: (i) The states of a system are represented by normalized vectors $|\Psi\rangle$ of a complex Hilbert space, and the observables are given by self-adjoint operators acting on this space. (ii) The expectation value of a measurable $\hat{A}$ at time t is $\bar{A}(t) = \langle\Psi(t)|\hat{A}|\Psi(t)\rangle$. (iii) The probability that a measurement of an observable $\hat{A}$ at time t yields A is $|\langle A|\Psi(t)\rangle|^2$, where $\hat{A}|A\rangle = A|A\rangle$. (iv) The state space of a composite system is the tensor product of the subsystems' state spaces. Having accepted these postulates, the rest—state spaces, observables, and the equations of motion—can be deduced directly from observable data. Importantly, these axioms are just the well-known quantum mechanical postulates with the adjective *quantum removed, as* $|\Psi\rangle$ is a general state encompassing classical and quantum behavior. We will demonstrate below that these postulates are sufficient to capture all the features of both quantum *and* classical mechanics as well as the associated hybrid mechanics. Equation (1) rewritten in terms of the axioms becomes

$$m\frac{d}{dt}\langle\Psi(t)|\hat{x}|\Psi(t)\rangle = \langle\Psi(t)|\hat{p}|\Psi(t)\rangle,$$
$$\frac{d}{dt}\langle\Psi(t)|\hat{p}|\Psi(t)\rangle = \langle\Psi(t)| - U'(\hat{x})|\Psi(t)\rangle. \qquad (2)$$

Koopman and von Neumann [7,8] pioneered the recasting of classical mechanics in a form similar to quantum mechanics by introducing classical complex valued wave functions and representing associated physical observables by means of commuting self-adjoint operators (for modern developments and applications see Refs. [9–23]). Our operational formulation is closely related to the approach proposed in Ref. [24] and recently successfully implemented for quantum state tomography [25,26]. Regarding the developments of other operational approaches see Ref. [27] and references therein.

Inference of classical dynamics.—Let $\hat{x}$ and $\hat{p}$ be self-adjoint operators representing the coordinate and momentum observables. The commutation relationship

$$[\hat{x}, \hat{p}] = 0 \qquad (3)$$

encapsulates two basic experimental facts of classical kinematics: (i) the position and momentum can be measured simultaneously with arbitrary accuracy, and (ii) observed values do not depend on the order of performing the measurements. In terms of our axioms, the dynamical observations of the classical particle's position and momentum are summarized in Eq. (2).

We now derive the equation of motion for a classical state. The application of the chain rule to Eq. (2) gives

$$\langle d\Psi/dt|\hat{x}|\Psi\rangle + \langle\Psi|\hat{x}|d\Psi/dt\rangle = \langle\Psi|\hat{p}/m|\Psi\rangle,$$
$$\langle d\Psi/dt|\hat{p}|\Psi\rangle + \langle\Psi|\hat{p}|d\Psi/dt\rangle = \langle\Psi| - U'(\hat{x})|\Psi\rangle, \qquad (4)$$

into which we substitute a consequence of Stone's theorem (see Sec. I of Ref. [3]),

$$i|d\Psi(t)/dt\rangle = \hat{L}|\Psi(t)\rangle, \qquad (5)$$

and obtain

$$im\langle\Psi(t)|[\hat{L}, \hat{x}]|\Psi(t)\rangle = \langle\Psi(t)|\hat{p}|\Psi(t)\rangle,$$
$$i\langle\Psi(t)|[\hat{L}, \hat{p}]|\Psi(t)\rangle = -\langle\Psi(t)|U'(\hat{x})|\Psi(t)\rangle. \qquad (6)$$

Since Eq. (6) must be valid for all possible initial states, the averaging can be dropped, and we have the system of commutator equations for the motion generator $\hat{L}$,

$$im[\hat{L}, \hat{x}] = \hat{p}, \qquad i[\hat{L}, \hat{p}] = -U'(\hat{x}). \qquad (7)$$

Since $\hat{p}$ and $\hat{x}$ commute, the solution $\hat{L}$ cannot be found by simply assuming $\hat{L} = L(\hat{x}, \hat{p})$ (regarding the definition of functions of operators see Sec. II of Ref. [3]). We add into consideration two new operators $\hat{\lambda}_x$ and $\hat{\lambda}_p$ such that

$$[\hat{x}, \hat{\lambda}_x] = [\hat{p}, \hat{\lambda}_p] = i, \qquad (8)$$

and the other commutators among $\hat{x}$, $\hat{p}$, $\hat{\lambda}_x$, and $\hat{\lambda}_p$ vanish. The need to introduce auxiliary operators arises in classical dynamics because all the observables commute; hence, the notion of an individual trajectory can be introduced (see also Sec. VIII in the Ref. [3]). Moreover, the choice of the commutation relationships (8) is unique. Equation (8) can be considered as an additional axiom. Now we seek the generator $\hat{L}$ in the form $\hat{L} = L(\hat{x}, \hat{\lambda}_x, \hat{p}, \hat{\lambda}_p)$. Utilizing Theorem 1 from Ref. [3], we convert the commutator equations (7) into the differential equations

$$mL'_{\lambda_x}(x, \lambda_x, p, \lambda_p) = p, L'_{\lambda_p}(x, \lambda_x, p, \lambda_p) = -U'(x), \qquad (9)$$

from which, the generator of classical dynamics $\hat{L}$ is found to be

$$\hat{L} = \hat{p}\hat{\lambda}_x/m - U'(\hat{x})\hat{\lambda}_p + f(\hat{x}, \hat{p}), \qquad (10)$$

where $f(x, p)$ is an arbitrary real-valued function. Equations (5), (8), and (10), represent classical dynamics in an abstract form.

Let us find the equation of motion for $|\langle px|\Psi(t)\rangle|^2$ by rewriting Eq. (5) in the xp representation (in which $\hat{x} = x$, $\hat{\lambda}_x = -i\partial/\partial x$, $\hat{p} = p$, and $\hat{\lambda}_p = -i\partial/\partial p$),

$$\left[i\frac{\partial}{\partial t} + i\frac{p}{m}\frac{\partial}{\partial x} - iU'(x)\frac{\partial}{\partial p} - f(x,p)\right]\langle px|\Psi(t)\rangle = 0, \tag{11}$$

which yields the well-known classical Liouville equation for the probability distribution in phase-space $\rho(x, p; t) = |\langle px|\Psi(t)\rangle|^2$,

$$\frac{\partial}{\partial t}\rho(x,p;t) = \left[-\frac{p}{m}\frac{\partial}{\partial x} + U'(x)\frac{\partial}{\partial p}\right]\rho(x,p;t). \tag{12}$$

Thus, we have deduced the classical Liouville equation along with the Koopman-von Neumann theory from Eq. (2) by assuming that the classical momentum and coordinate operators commute.

Inference of quantum dynamics.—The hallmark of quantum kinematics is the canonical commutation relation

$$[\hat{x}, \hat{p}] = i\hbar, \tag{13}$$

which implies (i) the Heisenberg uncertainty principle and (ii) the order of performing measurements of the coordinate and momentum does matter [6]. The evolution of expectation values of the quantum coordinate and momentum is governed by the Ehrenfest theorems (2).

We repeat the algorithm exercised in classical mechanics above. Substituting the definition of the motion generator $\hat{H}$ obtained from Stone's theorem (see Sec. I in Ref. [3]),

$$i\hbar|d\Psi(t)/dt\rangle = \hat{H}|\Psi(t)\rangle, \tag{14}$$

into Eq. (2), we obtain

$$im[\hat{H}, \hat{x}] = \hbar\hat{p}, \qquad i[\hat{H}, \hat{p}] = -\hbar U'(\hat{x}). \tag{15}$$

Assuming $\hat{H} = H(\hat{x}, \hat{p})$ and utilizing Theorem 1 Ref. [3], the commutation relations in Eq. (15) reduce to $mH'_p(x, p) = p$ and $H'_x(x, p) = U'(x)$. Whence, the familiar quantum Hamiltonian readily follows as

$$\hat{H} = \hat{p}^2/(2m) + U(\hat{x}). \tag{16}$$

Since the Schrödinger equation was derived from the Ehrenfest theorems (2), assuming the canonical commutation relation (13), the presentation suggests that the Ehrenfest theorems are more fundamental than the Schrödinger equation.

Unification of quantum and classical mechanics.—(For a detailed discussion see Sec. III in Ref. [3]; see also Fig. 2 therein for a graphical summary). The fundamental difference between nonrelativistic classical and quantum mechanics is that the momentum and coordinate operators commute in the former case and do not commute in the latter [28–30]. The operators $\hat{x}$, $\hat{p}$, $\hat{\lambda}_x$, and $\hat{\lambda}_p$ obeying Eq. (8) form the classical operator algebra. The unified quantum-classical operator algebra is based on $\hat{x}_q$, $\hat{p}_q$, $\hat{\vartheta}_x$, and $\hat{\vartheta}_p$ satisfying

$$[\hat{x}_q, \hat{p}_q] = i\hbar\kappa, \qquad [\hat{x}_q, \hat{\vartheta}_x] = [\hat{p}_q, \hat{\vartheta}_p] = i, \tag{17}$$

$0 \leq \kappa \leq 1$, while all the other commutators among $\hat{x}_q$, $\hat{p}_q$, $\hat{\vartheta}_x$, and $\hat{\vartheta}_p$ vanish. The operators $\hat{\vartheta}_x$ and $\hat{\vartheta}_p$ are simply introduced so that the quantum algebra (i.e., $\kappa = 1$) is consistent with the classical algebra. The limit $\kappa \to 0$ defines the quantum-to-classical transition with the quantum algebra smoothly transforming into the classical one as $\kappa \to 0$. Since $\hbar$ enters in the time derivative of the Schrödinger equation (14) as well as in the commutator relationship (13), the limit $\hbar \to 0$ encompasses more than the criterion that the coordinate and momentum operators must commute in the classical limit. This situation motivated the introduction of the parameter κ.

As the first step towards unification of both mechanics, we apply ODM to

$$\begin{aligned} m\frac{d}{dt}\langle\Psi(t)|\hat{x}_q|\Psi(t)\rangle &= \langle\Psi(t)|\hat{p}_q|\Psi(t)\rangle, \\ \frac{d}{dt}\langle\Psi(t)|\hat{p}_q|\Psi(t)\rangle &= \langle\Psi(t)| - U'(\hat{x}_q)|\Psi(t)\rangle, \end{aligned} \tag{18}$$

and obtain the Hamiltonian

$$\hat{\mathcal{H}} = \frac{1}{\kappa}\left[\frac{\hat{p}_q^2}{2m} + U(\hat{x}_q)\right] + F(\hat{p}_q - \hbar\kappa\hat{\vartheta}_x, \hat{x}_q + \hbar\kappa\hat{\vartheta}_p), \tag{19}$$

such that $i\hbar|d\Psi(t)/dt\rangle = \hat{\mathcal{H}}|\Psi(t)\rangle$, where F is an arbitrary real-valued smooth function. Note that no Ehrenfest theorems for the observables $\hat{O} = O(\hat{x}_q, \hat{p}_q)$ can specify the function F because $[\hat{F}, \hat{O}] = 0$. Hence, the function F is experimentally undetectable. We shall utilize this freedom by finding an F which enforces that the Hamiltonian (19) smoothly transforms to become the Liouvillian (10) in the classical limit.

The classical and quantum algebras are isomorphic. The quantum operators can be constructed as linear combinations of the classical operators in many ways, e.g.,

$$\begin{aligned} &\hat{x}_q = \hat{x} - \hbar\kappa\hat{\lambda}_p/2, \qquad \hat{p}_q = \hat{p} + \hbar\kappa\hat{\lambda}_x/2, \\ &\hat{\vartheta}_x = \hat{\lambda}_x, \qquad \hat{\vartheta}_p = \hat{\lambda}_p. \end{aligned} \tag{20}$$

In particular, demanding that the quantum operators are expressed as linear combinations of the classical ones such that

$$\begin{aligned} &\lim_{\kappa\to 0}\hat{x}_q = \hat{x}, \qquad \lim_{\kappa\to 0}\hat{p}_q = \hat{p}, \qquad \lim_{\kappa\to 0}\hat{\theta}_x = \hat{\lambda}_x, \\ &\lim_{\kappa\to 0}\hat{\theta}_p = \hat{\lambda}_p, \qquad \lim_{\kappa\to 0}\hat{\mathcal{H}} = \hbar\hat{L}, \end{aligned} \tag{21}$$

identifies the function F as (see Theorems 4 and 5 in Ref. [3])

$$F(p, x) = -p^2/(2m\kappa) - U(x)/\kappa + O(1). \quad (\kappa \to 0) \tag{22}$$

Keeping the leading term in Eq. (22), we show in Sec. III of Ref. [3] that only isomorphism (20) is compatible with such a function F, which leads to the final expression for the unified quantum-classical Hamiltonian,

$$\hat{\mathcal{H}}_{qc} = \frac{1}{\kappa}\left[\frac{\hat{p}_q^2}{2m} + U(\hat{x}_q)\right] - \frac{1}{2m\kappa}(\hat{p}_q - \hbar\kappa\hat{\vartheta}_x)^2 - \frac{1}{\kappa}U(\hat{x}_q + \hbar\kappa\hat{\vartheta}_p) \equiv \frac{\hbar}{m}\hat{p}\hat{\lambda}_x + \frac{1}{\kappa}U\left(\hat{x} - \frac{\hbar\kappa}{2}\hat{\lambda}_p\right) - \frac{1}{\kappa}U\left(\hat{x} + \frac{\hbar\kappa}{2}\hat{\lambda}_p\right). \quad (23)$$

that fulfills conditions (21). Theorem 6 in Ref. [3] states that $\hat{\mathcal{H}}_{qc} \equiv \hbar\hat{L}$ for any value of κ if and only if U is a quadratic polynomial.

We now demonstrate that the Wigner phase-space representation is a special case of the unified mechanics. First rewriting the equation of motion

$$i\hbar|d\Psi_\kappa(t)/dt\rangle = \hat{\mathcal{H}}_{qc}|\Psi_\kappa(t)\rangle \quad (24)$$

in the $x\lambda_p$ representation (for which $\hat{x} = x$, $\hat{\lambda}_x = -i\partial/\partial x$, $\hat{p} = i\partial/\partial\lambda_p$, and $\hat{\lambda}_p = \lambda_p$), then introducing new variables $u = x - \hbar\kappa\lambda_p/2$ and $v = x + \hbar\kappa\lambda_p/2$, we transform Eq. (24) into

$$\left[i\hbar\kappa\frac{\partial}{\partial t} - \frac{(\hbar\kappa)^2}{2m}\left(\frac{\partial^2}{\partial v^2} - \frac{\partial^2}{\partial u^2}\right) - U(u) + U(v)\right]\rho_\kappa = 0,$$

where $\rho_\kappa(u, v; t) \propto \langle x\lambda_p|\Psi_\kappa(t)\rangle$. Therefore, ρ_κ is the density matrix for a quantum system with the Hamiltonian (16) after substituting $\hbar \to \hbar\kappa$. Note that κ enters the equation of motion (24) as only a multiplicative constant renormalizing $\hbar$. From this perspective, the limit $\kappa \to 0$ is indeed equivalent to $\hbar \to 0$. The transition from the $x\lambda_p$ to xp representation results in

$$\langle px|\Psi_\kappa(t)\rangle = \sqrt{\frac{\hbar\kappa}{2\pi}}\int d\lambda_p \rho_\kappa\left(x - \frac{\hbar\kappa\lambda_p}{2}, x + \frac{\hbar\kappa\lambda_p}{2}; t\right)e^{ip\lambda_p}. \quad (25)$$

Hence, the wave function $\langle px|\Psi_\kappa(t)\rangle$ is proportional to the celebrated Wigner quasiprobability distribution.

By only demanding a consistent melding of quantum and classical mechanics within ODM, we achieved the construction equivalent to the Wigner phase-space formulation of quantum mechanics. The great attraction of the Wigner formalism is due to its smooth and physically consistent quantum-to-classical and classical-to-quantum transitions [29–36]. Our analysis also points to a unique feature of the phase-space formulation: no quantum mechanical representation, but Wigner's, has a *nice* classical limit. Moreover, since the Wigner function's dynamical equation is recast in the form of a Schrödinger-like equation (24), efficient numerical methods for solving the Schrödinger equation may be applied to propagate the Wigner function for conceptual appeal and practical utility.

Future prospects.—ODM was introduced to derive equations of motion from the evolution of average values and a chosen kinematical description. In Secs. IV–IX of Ref. [3], ODM is applied to the canonical quantization rule, the Schwinger quantum action principle, the time measuring problem in quantum mechanics, quantization in curvilinear coordinates, as well as classical and quantum field theories. Additionally, relativistic classical and quantum mechanics is also melded within this framework in Ref. [37].

Variational principles are at the heart of physics. Within their framework, the problem of model generation is reduced to finding the correct form of the action functional, whose Euler-Lagrange equations govern the model's dynamics. However, the action is usually neither directly observable nor unique; hence, its construction is a subject of debate and can only be justified *postfactum* by supplying experimentally verifiable equations of motion. More importantly, there are phenomena beyond the scope of variational principles (e.g., dissipation). ODM is a theoretical framework free of all these conceptual weaknesses since it operates with observable data recast in the form of Ehrenfest-like relations. Hence, the equations of motion are no longer axioms but are corollaries of the more fundamental Ehrenfest theorems.

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