

The History of Hilbert-Space Formulations of Classical Physics

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Abstract

Hilbert-space techniques are widely used not only for quantum theory, but also for classical physics. Two important examples are the Koopman-von Neumann (KvN) formulation and the method of “classical” wave functions. As this paper explains, these two approaches are conceptually distinct. In particular, the method of classical wave functions was not due to Bernard Koopman and John von Neumann, but was developed independently by a number of later researchers, perhaps first by Mario Schönberg, with key contributions from Angelo Loinger, Giacomo Della Riccia, Norbert Wiener, and E. C. George Sudarshan. The primary goals of this paper are to explain these two approaches, describe the relevant history in detail, and give credit where credit is due.

1 Introduction

In 1931, Bernard Koopman published a paper titled “Hamiltonian Systems and Transformations in Hilbert Space” in the *Proceedings of the National Academy of Sciences* (Koopman 1931). Koopman’s paper laid out a novel method for identifying functions representing observables on a classical system’s phase space as vectors in a new kind of Hilbert space. In 1932, John von Neumann published a pair of follow-up papers in German in *Annals of Mathematics* (von Neumann 1932a, 1932b) further developing Koopman’s method.

Koopman’s use of Greek letters for his phase-space functions may have made it easy to confuse them with classical versions of the state vectors or wave functions of quantum mechanics, and von Neumann’s two papers were never translated into English. Koopman and von Neumann’s papers, however, did not refer to classical state vectors or wave functions, and their Hilbert spaces consisted of functions representing classical observables, which naturally corresponded to quantum-mechanical operators evolving in time in the Heisenberg picture. Indeed, as Jordan and Sudarshan noted in a 1961 paper published in the *Journal of Mathematical Physics*:

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It was shown by Koopman how the dynamical transformations of classical mechanics, considered as measure preserving transformations of the phase space, induce unitary transformations on the Hilbert space of functions which are square integrable with respect to a density function over the phase space. This Hilbert space formulation of classical mechanics was further developed by von Neumann. It is to be noted that this Hilbert space corresponds not to the space of state vectors in quantum mechanics but to the Hilbert space of operators on the state vectors (with the trace of the product of two operators being chosen as the scalar product). [Jordan, Sudarshan 1961, pp. 515–516]

Danilo Mauro wrote an innovative and influential 2002 paper titled “On Koopman-von Neumann Waves” (Mauro 2002), later expanding on his work in his 2003 PhD thesis, titled “Topics in Koopman-von Neumann Theory” (Mauro 2003). The paper and thesis replaced the observables-as-vectors method described above with an important but different technique. This different technique was to use complex-valued “classical” wave functions ψ in place of classical probability distributions ρ , where these classical wave functions and classical probability distributions were explicitly related by the modulus-square operation, $\rho = |\psi|^2$, in analogy with the Born rule. However, this method of classical wave functions was due to other researchers who came decades after Koopman and von Neumann’s papers from the 1930s—perhaps the first being Mario Schönberg, working in the 1950s.

Ever since this accidental misattribution, the “Koopman-von Neumann (KvN) formulation” has been widely but incorrectly employed to refer to the method of classical wave functions. For example, an international conference in 2021 and an accompanying special issue of *Journal of Physics A* in 2022, both titled “Koopman Methods in Classical and Classical-Quantum Mechanics,” referred in their abstracts to “Koopman-von Neumann wave functions” (Bondar et al, 2021, 2022). As of the writing of this paper, the Wikipedia entry “Koopman-von Neumann Classical Mechanics” (Wikipedia 2025) opens up its derivation of the framework with the following statement:

In the approach of Koopman and von Neumann (KvN), dynamics in phase space is described by a (classical) probability density, recovered from an underlying wavefunction—the Koopman-von Neumann wavefunction—as the square of its absolute value (more precisely, as the amplitude multiplied with its own complex conjugate).

The main purpose of the present paper is to lay out the detailed history of both the Koopman-von Neumann formulation and the method of classical wave functions, and assign credit appropriately.

Ultimately, it turns out that the Hilbert spaces that arise from treating observables as vectors and the Hilbert spaces that arise from classical wave functions are mathematically equivalent. This equivalence between the two kinds of Hilbert spaces is an elementary result of the GNS construction (Gelfand, Naimark 1943; Segal 1947), which takes the elements f, g, \dots of a C*-algebra (representing observables) together with a positive, normalized linear functional ω in the dual space of the C*-algebra (representing quantum states), and combines them to form a rudimentary inner product $(f, g) \equiv \omega(f^*g)$ that eventually underwrites the definition of a Hilbert space representing the original C*-algebra. However, despite this underlying connection between, on the one hand, the original observables-as-vectors method of Koopman and von Neumann, and, on the other hand, the

classical-wave-function method that came later, these are conceptually different methods. Simply put, Koopman and von Neumann did not come up with the idea of using classical wave functions to capture classical probability distributions.

By analogy, Heisenberg’s matrix mechanics (Heisenberg 1925) and Schrödinger’s wave mechanics (Schrödinger 1926) were conceptually different frameworks. It was Schrödinger who came up with the idea of quantum-mechanical wave functions, and it would not be correct to give credit to Heisenberg for that idea, even though matrix mechanics and wave mechanics were eventually connected to each other by modern Hilbert-space formulations of quantum theory.

2 Hilbert-Space Formulations of Classical Physics

2.1 Bernard Koopman

Koopman began his 1931 paper with the following motivation:

In recent years the theory of Hilbert space and its linear transformations has come into prominence. [...] It is the object of this note to outline certain investigations of our own in which the domain of this theory has been extended in such a way as to include classical Hamiltonian mechanics, or, more generally, systems defining a steady n -dimensional flow of a fluid of positive density. [Koopman 1931, p. 315]

Shortly thereafter, Koopman described his basic approach:

The starting point of our investigation is the N -dimensional variety Ω and the group of automorphisms S_t having the positive integral invariant $\int \rho d\omega$, and these are considered without reference to the problem which gave them origin. Let $\varphi = \varphi(A)$ be a complex-valued function of the point A of Ω , restricted only as follows: (i) φ is single-valued; (ii) φ is measurable; (iii) the Lebesgue integrals $\int_{\Omega} \rho |\varphi| d\omega$ and $\int_{\Omega} \rho |\varphi|^2 d\omega$ are finite. The totality of such functions φ constitutes the aggregate of points of a Hilbert space \mathfrak{H} : the metric of which is determined by the “inner product”

$$(\varphi, \psi) = \int_{\Omega} \rho \varphi \bar{\psi} d\omega. \tag{1}$$

[Ibid., p. 316]

Notice the function ρ appearing in Koopman’s integral measures, separate from the functions φ and ψ . As Koopman wrote, “here, ρ is a positive, single-valued, analytic function on Ω . This is a consequence of the fact that $\int dq_1 \dots dq_n dp_1 \dots dp_n$ is an integral invariant of the system” (Ibid., p. 315). Later, Koopman added: “If t represents the time, S_t specifies the steady flow of a fluid of density ρ occupying the space Ω ” (Ibid., p. 316). After introducing Gaussian coordinates ξ_1, \dots, ξ_N , with corresponding velocities $\Xi_k = d\xi_k/dt$, Koopman wrote:

The property of $\rho = \rho(\xi_1, \dots, \xi_N)$ is expressed by the “equation of continuity”

$$\sum_{k=1}^N \frac{\partial(\rho \Xi_k)}{\partial \xi_k} = 0. \quad (2)$$

These statements make clear that Koopman’s functions φ and ψ were not related to probability densities, and that his density function ρ was a separate mathematical object that partly defined Koopman’s Hilbert space. Koopman did not suggest that his functions φ and ψ should include classical wave functions, or be related to a probability density by the modulus-squaring operation.

In Koopman’s paper, he defined the time evolution of his functions φ, ψ, \dots using a transformation U_t defined by

$$U_t \varphi(A) \equiv \varphi(S_t A), \quad (3)$$

where A is a given phase-space point and where $S_t A$ is the new phase-space point after a duration t of classical Hamiltonian time evolution. Working in coordinates for the given $2n$ -dimensional phase space, so that one can denote a phase-space point as $A = (q, p) \equiv (q_1, \dots, q_n; p_1, \dots, p_n)$, one has a coordinate representation of Koopman’s notion of time evolution,

$$S_t(q, p) \equiv (q(t), p(t)), \quad (4)$$

and so $U_t \varphi(A)$ has time derivative given by

$$\begin{aligned} \frac{d}{dt} U_t \varphi(A) &= \frac{d}{dt} \varphi(S_t A) \\ &= \frac{d}{dt} \varphi(q(t), p(t)) \\ &= \sum_{k=1}^n \frac{\partial \varphi}{\partial q_k} \frac{dq_k(t)}{dt} + \sum_{k=1}^n \frac{\partial \varphi}{\partial p_k} \frac{dp_k(t)}{dt} \\ &= \sum_{k=1}^n \left(\frac{\partial \varphi}{\partial q_k} \frac{\partial H}{\partial p_k} - \frac{\partial \varphi}{\partial p_k} \frac{\partial H}{\partial q_k} \right) \\ &= \{\varphi, H\}, \end{aligned}$$

which is the appropriate time-evolution equation for a function representing a classical observable, with $\{\varphi, H\}$ the usual Poisson bracket of φ and H . Introducing the standard formula for the Liouvillian operator L ,

$$L \equiv i\{H, \} \equiv i \sum_{k=1}^n \left(\frac{\partial H}{\partial q_k} \frac{\partial}{\partial p_k} - \frac{\partial H}{\partial p_k} \frac{\partial}{\partial q_k} \right), \quad (5)$$

one can recast the time-evolution equation for φ as¹

$$\frac{d}{dt}U_t\varphi(A) = \{\varphi, H\} = iL\varphi. \quad (6)$$

By contrast, under the time evolution $S_t(q, p) \equiv (q(t), p(t))$ expressed in (4), a time-dependent probability density $\rho(q, p, t)$ on the classical phase space should evolve instead according to the classical Liouville equation:

$$\frac{\partial \rho}{\partial t} = \{H, \rho\} = -iL\rho. \quad (7)$$

Because the Liouvillian operator (5) involves only first-order derivatives, the same should be true of any classical wave function ψ whose modulus-square is ρ .

Finally, for the case of a probability density ρ without any explicit time-dependence, the classical Liouville equation reduces to

$$\{H, \rho\} = 0,$$

which implies that

$$\sum_{k=1}^n \frac{\partial \rho}{\partial q_k} \frac{dq_k(t)}{dt} + \sum_{k=1}^n \frac{\partial \rho}{\partial p_k} \frac{dp_k(t)}{dt} = 0,$$

exactly in keeping with Koopman's continuity equation (2). These results confirm that Koopman's function ρ really does correspond most closely with a classical system's probability density, and is conceptually distinct from Koopman's phase-space functions φ, ψ, \dots

From Koopman's notion of time evolution, (3), one can see at an even deeper level why his phase-space functions were not akin to wave functions. For any classical phase-space point A , let ω_A be a positive linear functional acting on Koopman's functions φ, ψ, \dots according to

$$\omega_A(\varphi) \equiv \varphi(A), \quad (8)$$

and satisfying the usual desiderata of a state map in the C*-algebraic sense. For any time t , let g_t be the map acting on ω_A by replacing A with its time-evolved counterpart $S_t A$, in accordance with Koopman's notion of time evolution:

$$g_t \omega_A \equiv \omega_{S_t A}. \quad (9)$$

It follows immediately that

$$(g_t \omega_A)(\varphi) = \omega_A(U_t \varphi). \quad (10)$$

Evidently, the time evolution of state maps ω_A is opposite to the time evolution of functions φ , in an abstraction of the usual distinction between Schrödinger-picture time evolution and Heisenberg-

¹Koopman wrote in his paper that "if the values of $\varphi(A)$ be regarded as being attached to the respective points A of the fluid when $t = 0$, in the course of the flow these values will be carried into those of the function $U_{-t}\varphi(A)$ " (Koopman 1931, p. 316). This picture led Koopman to calculate instead $[(\partial/\partial t)U_t\varphi(A)]_{t=0} = iP\varphi(A)$, where P differed by an overall sign from the usual definition of the Liouvillian operator L in (5). Koopman's equation, however, was not a time-evolution equation in the usual sense of describing the behavior of a given function at arbitrary times t . Instead, Koopman treated his equation merely as a mathematical step toward writing down a self-adjoint generator P for his transformation U_t .

picture time evolution. According to Koopman's transformation U_t , his phase-space functions time-evolve as Heisenberg-picture observables, not as Schrödinger-picture wave functions.

2.2 John von Neumann

Koopman did not mention wave functions at all in his paper. By contrast, von Neumann did mention wave functions, but only in the first of his two 1932 papers (von Neumann 1932a), and only to suggest an analogy between Koopman's time-evolution operator U_t and the time evolution appearing in quantum mechanics:

Finally, we would like to point out the interesting analogy between Koopman's operators $U_t = e^{itA}$ and the operators of quantum mechanics. The Schrödinger wave function φ (defined in the state space of the mechanical system and not like our f in phase space!) obeys, as is well known, in its dependence on the time parameter t the differential equation $\frac{h}{2\pi i} \frac{\partial \varphi}{\partial t} = H\varphi$. Here h is Planck's quantum of action and H the energy operator. From this it follows at once $\varphi = e^{it \cdot \frac{2\pi}{h} H} \varphi_{(t=0)}$ [footnote in the original: This relationship is usually written with $-H$ instead of H .], so that here the unitary operators $\hat{U}_t = e^{it \cdot \frac{2\pi}{h} H}$ play a fundamental role. The analogy, which arises from the juxtaposition of A and $\frac{2\pi}{h} H$, is striking [footnote in the original: A closer look shows that it becomes more perfect if one replaces the differential equation of the wave function with that of the so-called statistical operator (cf., for example, J. v. Neumann, *Mathematische Grundlagen der Quantenmechanik*, Berlin 1932, p. 186). However, it is constructed in the same way, and what will be said below also applies to it.], and it is even possible to exhibit the continuous passage of quantum mechanics into the classical (as $h \rightarrow 0$). Nevertheless, there seem to be essential mathematical differences between these two families of operators. For a mechanical system confined to a finite volume, quantum mechanics always appears to exhibit a pure point spectrum, whereas in the classical-mechanical problem a pure continuous spectrum seems to be the generic case (cf. § VI). [Ibid., pp. 594-595]²

²In the original German:

Zum Schluß sei noch auf die interessante Analogie zwischen Koopmans Operatoren $U_t = e^{itA}$ und den Operatoren der Quantenmechanik hingewiesen. Die Schrödingersche Wellenfunktion φ (definiert im Zustandsraum des mechanischen Systems und nicht wie unsere f im Phasenraum!) gehorcht bekanntlich in ihrer Abhängigkeit vom Zeitparameter t der Differentialgleichung $\frac{h}{2\pi i} \frac{\partial \varphi}{\partial t} = H\varphi$. Hier ist h das Plancksche Wirkungsquantum und H der Energieoperator. Hieraus folgt sofort $\varphi = e^{it \cdot \frac{2\pi}{h} H} \varphi_{(t=0)}$ [Meistens wird diese Beziehung mit $-H$ statt H geschrieben], so daß hier die unitären Operatoren $\hat{U}_t = e^{it \cdot \frac{2\pi}{h} H}$ eine fundamentale Rolle spielen. Die Analogie, die durch das Nebeneinanderstellen von A und $\frac{2\pi}{h} H$ entsteht, ist auffallend [Eine genauere Überlegung zeigt, daß sie vollkommener wird, wenn man die Differentialgleichung der Wellenfunktion durch diejenige des sog. statistischen Operators ersetzt (vgl. z. B. J. v. Neumann, *Mathematische Grundlagen der Quantenmechanik*, Berlin 1932, S. 186). Dieselbe ist aber ebenso gebaut und das weiter unten zu Sagende gilt auch für sie.], und es ist möglich, sie zum Nachweis des stetigen Übergangs der Quantenmechanik in die klassische (für $h \rightarrow 0$) auszubauen. Trotzdem scheinen wesentliche mathematische Unterschiede zwischen diesen Operatorenscharen zu bestehen. Denn für ein mechanisches System, das in ein endliches Volumen eingesperrt ist, scheint in der Quantenmechanik stets ein reines Punktspektrum vorzuliegen, während im klassisch-mechanischen Problem das reine Strecken-

Notice the footnote in which von Neumann pointed out that his phase-space function f should evolve under $-H$ rather than H . Once again, this reversed time evolution is due to f being akin to an observable, and not a wave function.

2.3 Mario Schönberg

In the early 1950s, Mario Schönberg published a pair of papers in *Il Nuovo Cimento* (Schönberg 1952, 1953) in which he introduced the method of classical wave functions, an idea that did not appear in the 1930s papers by Koopman or von Neumann. Again, a classical wave function is a complex-valued function whose modulus-square gives the probability density for a classical system.

Following Schönberg and his notation, he considered a system of n particles with positions $\mathbf{x}_1, \dots, \mathbf{x}_n$ and momenta $\mathbf{p}_1, \dots, \mathbf{p}_n$, as well as a probability density f_n . Schönberg called his new complex-valued function Θ_n , and then his equation (10) from his 1952 paper took the form:

$$f_n(\mathbf{x}_1, \dots, \mathbf{x}_n; \mathbf{p}_1, \dots, \mathbf{p}_n) = |\Theta_n(\mathbf{x}_1, \dots, \mathbf{x}_n; \mathbf{p}_1, \dots, \mathbf{p}_n)|^2 \quad [\text{Schönberg's eq. (16)}]. \quad (11)$$

Earlier in his paper, in his equation (8), Schönberg had noted that the probability density f_n obeyed the classical Liouville equation, in accord with (7),

$$\frac{\partial f_n}{\partial t} = (H_n, f_n)_n = -iL_n f_n \quad [\text{Schönberg's eq. (8)}], \quad (12)$$

where L_n is the n -particle Liouville operator, and where Schönberg used the following notation for Poisson brackets:

$$(F, G)_n = \sum_{l=1}^n \left\{ \frac{\partial F}{\partial \mathbf{x}_l} \frac{\partial G}{\partial \mathbf{p}_l} - \frac{\partial F}{\partial \mathbf{p}_l} \frac{\partial G}{\partial \mathbf{x}_l} \right\} \quad [\text{Schönberg's eq. (9)}]. \quad (13)$$

As Schönberg then explained, “since the square of the absolute value of a solution of the Liouville equation is also a solution of the same equation,” it followed that his new complex-valued function Θ_n satisfied the same equation:

$$\frac{\partial \Theta_n}{\partial t} = (H_n, \Theta_n)_n = -iL_n \Theta_n \quad [\text{Schönberg's eq. (17)}]. \quad (14)$$

In the paragraph that followed this equation, Schönberg wrote:

Thus we are led to a kind of wave function in classical statistical mechanics. Equation (17) may be considered as the classical wave equation, the [H]ermitian operator L_n playing the part of [a] classical [H]amiltonian operator. [Schönberg 1952, p. 1142]

In the opening of his 1953 paper, Schönberg wrote:

spektrum der allgemeine Fall zu sein scheint (vgl. § VI).

In the preceding part of [Schönberg 1952] we have shown that it is possible to develop in the classical mechanics a wave formalism in phase space which presents many of the features of the quantum wave mechanics. [...] [W]e may introduce a wave function $\Theta(q, p)$, in general complex, such that the probability density be the square of its absolute value:

$$f(q, p) = |\Theta(q, p)|^2 \quad [\text{Schönberg's eq. (3)}]. \quad (15)$$

The consideration of the wave function gives some essential new possibilities, because it is not restricted to have only real and positive values, as the probability density. [Schönberg 1953, p. 419]

In that 1953 paper, Schönberg made only a single reference to Koopman's 1931 paper, pointing to the underlying mathematical equivalence between Schönberg's Hilbert spaces and Koopman's Hilbert spaces that was described in Section 1 of the present paper:

The introduction of the classical functions clarifies the meaning of the unitary transformations in Hilbert space associated with the motion of a classical system, which were introduced by Koopman. The Koopman Hilbert-space can be taken as that of the classical wave functions. [Schönberg 1953, p. 425]

It is unclear whether Schönberg meant something more by these remarks, such as asserting not just a correspondence between underlying Hilbert spaces, but a closer relationship between his classical wave functions and Koopman's phase-space functions. The answer may be lost to history.

2.4 Angelo Loinger

In 1962, Angelo Loinger published a paper titled “Galilei Group and Liouville Equation” in *Annals of Physics* (Loinger 1962). The paper explicitly distinguished between the original Koopman-von Neumann construction and Schönberg's work. In his introduction, Loinger wrote:

In Section I the Hilbert space formulation of classical mechanics, according to the viewpoints developed respectively by Koopman and by Schönberg, is briefly reviewed in a convenient form and the intimate relationship existing between the two conceptions is pointed out. [Ibid., p. 132]

Loinger then went on to review the original Koopman-von Neumann approach in Section I.A. of the paper (“Preliminaries and Koopman's Viewpoint”). In that section, Loinger slightly altered the definition of the inner product (1), writing:

We then consider the Hilbert space \mathfrak{K} of the complex square integrable functions $f(\omega)$ of the points of Ω_{2n} [the classical system's $2n$ -dimensional phase space], in which an inner product is defined as follows:

$$(f, g) \stackrel{\text{Def.}}{=} \int_{\Omega} f^*(\omega) g(\omega) d\omega \quad [\text{Loinger's eq. (9)}]. \quad (16)$$

[Ibid., p. 134]

Note the absence of the phase-space probability density ρ in this definition, as compared with Koopman’s original definition (1). Loinger then wrote:

We put, with a bra and ket notation:

$$(f, g) \equiv (f|g) \quad [\text{Loinger’s eq. (11)}] \quad (17)$$

and consider the extension \mathfrak{K}_D of \mathfrak{K} in Dirac’s sense. [Ibid., p. 134]

Next, Loinger turned to a review of Schönberg’s framework in Section II.A (“Schönberg’s Viewpoint”), writing:

The formulation of the classical mechanics given in Section I, A is formally analogous to a formulation of quantum mechanics, which was first studied by von Neumann. In this von Neumann quantal scheme the operators of the conventional formulation are considered as vectors of a new Hilbert space. One may ask whether even in the classical case it is possible to introduce a Hilbert space, say \mathfrak{H}_D , analogous to the state-vector space of quantum mechanics. It can easily be seen that such a space exists and stays in a very simple relationship with \mathfrak{K}_D . [Ibid., pp. 134–135]

Loinger added parenthetically that he would show later that the two Hilbert spaces were mathematically equivalent, writing:

(Actually, as will be apparent presently, \mathfrak{H}_D and \mathfrak{K}_D are the same space.) [Ibid., p. 135]

However, throughout the paper, Loinger emphasized that despite the isomorphism between \mathfrak{H}_D and \mathfrak{K}_D , they had conceptually different meanings. For example, he included the following additional parenthetical note:

(We distinguish here the vectors of \mathfrak{K}_D from those of \mathfrak{H}_D , reserving for the first ones the bra and ket notation with round parentheses.) [Ibid., p. 135]

2.5 Giacomo Della Riccia and Norbert Wiener

In 1966, the *Journal of Mathematical Physics* published a paper by Giacomo Della Riccia and (posthumously)³ Norbert Wiener (Della Ricci, Wiener 1966), titled “Wave Mechanics in Classical Phase Space, Brownian Motion, and Quantum Theory.” In their abstract, the authors wrote:

³The paper included the following note, at the end of its introductory section: “Because of the sad demise of Norbert Wiener in March 1964, the treatment given in this paper is due to the first-named author. For the same reason it seemed desirable that the results should be presented, however incomplete they may be.”

A wave dynamics of fields $\varphi(p, q; t) \in L_2(\Gamma)$ over the phase space $\Gamma(p, q)$ of a classical system \mathcal{S} is derived from the Liouville theorem. [...] From this it follows that we can regard normalized fields $\varphi(p, q; t)$ as “probability amplitudes” leading to a probability density function $\rho(p, q; t) = \varphi\varphi^*$ in the sense of Gibbs’ statistical mechanics. [Ibid., p. 1372]

In their introductory material, Della Riccia and Wiener wrote:

In Gibbs statistical mechanics the basic quantity is a probability density function $\rho(p, q; t)$ defined over the phase space of the mechanical system \mathcal{S} under observation. In our work we introduce in phase space a new quantity $\varphi(p, q; t)$, which by definition is a normalized square-integrable, real, or complex-valued function. We call it a “probability amplitude” field. $\varphi(p, q; t)$ is required to satisfy the usual equation of continuity derived from the Liouville theorem.

[...]

In the last part of our work we are concerned with the problem of constructing probabilities out of “probability amplitudes.” We use known results based on Wiener’s mathematical theory of Brownian motion to derive probabilities which agree with those obtained from Born’s statistical postulate. The desired result is that it is possible to interpret the quantity $\rho(p, q; t) = \varphi\varphi^*$ as a probability density in the sense of Gibbs. [Ibid., pp. 1372–1373]

Della Riccia and Wiener made no mention of the 1930s papers by Koopman or von Neumann, nor did they cite Schönberg or Loinger. It may be that they did not see a connection between their classical probability amplitudes and the Koopman-von Neumann formulation, and might not have been aware of Schönberg and Loinger’s papers. Nevertheless, Della Riccia and Wiener recapitulated Schönberg’s derivation of the time-evolution equation (14), which they wrote as

$$-i(\partial\varphi/\partial t) = \mathcal{L}\varphi, \quad \varphi \in L_2 \quad [\text{Della Riccia and Wiener’s eq. (4)}], \quad (18)$$

with their Liouville operator defined, as usual, according to $\mathcal{L} = i[H, \cdot]$, where the right-hand side is Della Riccia and Wiener’s notation for the Poisson bracket with the Hamiltonian H .

2.6 E. C. George Sudarshan

In 1976, E. C. George Sudarshan laid out a very similar method in a paper published in the journal *Pramana*, titled “Interaction between Classical and Quantum Systems and the Measurement of Quantum Observables” (Sudarshan 1976). In the paper, Sudarshan described his motivation as trying to find a better way to capture how classical systems and quantum systems could interact with each other, especially during a measurement process. In Sudarshan’s own words:

I introduce a direct method of dealing with the interaction of classical and quantum systems. It is made possible by the discovery that a classical system can be embedded in a quantum system with a continuum of superselection sectors. [Ibid., p. 118]

In the second section of his paper, in defining a “quantum system” with this continuum of superselection sectors, whose eventual purpose was to represent a classical system with canonical coordinates $\omega = (x, p)$, Sudarshan wrote:

State vectors for the quantum system are given, in the Schrödinger representation, by their wave functions $\psi(\omega)$. But because of the superselection principle, the relative phase of the distinct ideal eigenstates of coordinate operators is unmeasurable and, therefore, irrelevant. Hence, we are led to the equivalence

$$\psi(\omega) \sim \psi(\omega) \exp\{i\phi(\omega)\} \quad [\text{Sudarshan's eq. (2.8)}]. \quad (19)$$

Therefore, only the absolute value of $\psi(\omega)$ is relevant and may be taken as the positive square root of the phase space density

$$\psi(\omega) = \sqrt{\rho(\omega)} \quad [\text{Sudarshan's eq. (2.9)}]. \quad (20)$$

The ideal eigenstates of the coordinate operators is [sic] identified with the classical state corresponding to a point in phase space. [Ibid., p. 120]

Crucially, Sudarshan included the following bracketed note:

[This construction of a quantum theory embedding the classical theory is to be contrasted with the work of Coopman [sic] 1931; see also, Jordan and Sudarshan 1961]. [Ibid., p. 120]

Sudarshan did not cite von Neumann, Schönberg, Loinger, Della Riccia, or Wiener in his paper. In a later paper that further developed these methods, published in *Physical Review D* in 1978, Sudarshan and his co-author, Tom Sherry, left out those names again, and did not cite Koopman, either (Sherry, Sudarshan 1978). Sudarshan was clearly familiar with von Neumann’s work, as the first of von Neumann’s 1932 papers was cited in Sudarshan’s earlier 1961 paper with Jordan (Jordan, Sudarshan 1961), as quoted in Section 1 of the present paper. Perhaps the other papers were simply unknown to Sudarshan at the time.

2.7 Ennio Gozzi

Danilo Mauro’s PhD supervisor at the University of Trieste was Ennio Gozzi. Gozzi had been working on formal connections between classical mechanics and quantum theory as far back as 1988, when he published a paper in *Physical Letters B*, titled “Hidden BRS Invariance in Classical Mechanics,” in which he derived a path-integral representation of classical mechanics (Gozzi 1988). In that paper, Gozzi also introduced a classical probability distribution on phase space, writing, in a footnote, “I owe this idea to a crucial discussion with E. [Erhard] Seiler.” As Gozzi wrote:

This classical path-integral formalism has, as the quantum one, a parallel operatorial version that is already well known. It is the Liouville version of classical mechanics in

which one introduces a classical probability density $\rho(p, q)$ which evolves in time as any other classical observables

$$\frac{\partial \rho}{\partial t} = \{\rho, H\}_{PB}, \quad (21)$$

where $\{P, B\}_{PB}$ are the usual Poisson brackets and H the [H]amiltonian. This equation can be put in the form

$$\frac{\partial \rho}{\partial t} = \hat{L}\rho \quad [\text{Gozzi's eq. (6)}], \quad (22)$$

where

$$\hat{L} = \frac{\partial H}{\partial p} \frac{\partial}{\partial q} - \frac{\partial H}{\partial q} \frac{\partial}{\partial p}, \quad (23)$$

which is known as the Liouville operator (Liouville). [Ibid., p. 526]

In this paper, Gozzi did not cite any of the authors discussed in the present work—Koopman, von Neumann, Schönberg, Loinger, Della Riccia, Wiener, or Sudarshan.

Gozzi first brought up links between these path-integral representations of classical mechanics and the methods of Koopman and von Neumann in a follow-up paper in *Physical Review D* in 1989, titled “Hidden BRS Invariance in Classical Mechanics. II” and co-authored with Martin Reuter and William Thacker (Gozzi, Reuter, Thacker 1989). Starting with this 1989 paper, Gozzi began citing Koopman’s papers and von Neumann’s papers, but, again, without any mention of classical wave functions. In the abstract, Gozzi and his co-authors wrote:

Associated with this path integral there is an operatorial formalism that turns out to be an extension of the well-known operatorial approach of Liouville, Koopman, and von Neumann. [Ibid., p. 3363]

In listing the virtues of Gozzi’s path-integral formulation of classical mechanics, the authors included:

Second, long ago Koopman and von Neumann, influenced by the invention of quantum mechanics, gave an *operatorial* formulation of CM [classical mechanics]. [Ibid., p. 3363, emphasis in the original]

Later on, the authors wrote:

The crucial elements of the operatorial formalism mentioned above are the “classical commutation relations” which follow from the classical path integral. This formalism naturally embeds the standard operator approach to CM pioneered by Liouville, Koopman and von Neumann. [Ibid., p. 3364]

In these papers in the late 1980s and well into the 1990s, Gozzi consistently referred to Koopman and von Neumann’s method quite reasonably as “the operatorial approach to classical mechanics.”

Gozzi began writing papers with Danilo Mauro in the late 1990s, starting with a preprint extending Gozzi’s work on path-integral representations of classical mechanics. This preprint appeared on the arXiv on July 9, 1999, and was eventually published in the *Journal of Mathematical Physics* in

2000 (Gozzi, Mauro 2000). The paper began with the following introductory statement, which remained fully in keeping with Gozzi’s phrasing of Koopman and von Neumann’s methods as providing an “operatorial” approach to classical mechanics:

Some time ago a *path-integral* formulation of classical mechanics (CM) appeared in the literature. This formulation was nothing else than the path-integral counterpart of the *operatorial* version of CM provided long ago by Koopman and von Neumann. [Ibid., p. 1916, emphasis in the original]

As with Gozzi’s previous papers, this paper did not mention classical wave functions.

Shortly thereafter, Gozzi and Mauro co-authored their next manuscript, this time with Enrico Deotto. The preprint was titled “Supersymmetry in Classical Mechanics” and showed up on the arXiv on January 18, 2001. It was published as part of a book, *A Concise Encyclopaedia of Supersymmetry*, in 2003 (Deotto, Gozzi, Mauro 2003). The article began with the following statements:

In 1931 Koopman and von Neumann proposed an *operatorial* formulation of Classical Mechanics (CM) expanding earlier work of Liouville. Their approach is basically the following: given a dynamical system with a phase space \mathcal{M} labelled by coordinates $\varphi^a = (q^i, p^i)$; $a = 1, \dots, 2n$; $i = 1, \dots, n$, with Hamiltonian H and symplectic matrix ω^{ab} , the evolution of a probability density $\rho(\varphi)$ can be given either via the Poisson brackets $\{ , \}$ or via the Liouville operator:

$$\frac{\partial \rho}{\partial t} = \{H, \rho\} = -\hat{L}\rho; \quad \hat{L} = \omega^{ab} \partial_b H \partial_a \quad [\text{Deotto, Gozzi, and Mauro’s eq. (1)}]. \quad (24)$$

The evolution via the Liouville operator is basically what is called the operatorial approach to CM. The natural question to ask is whether we can associate to the *operatorial* formalism of CM a *path integral* one, like it is done in quantum mechanics. The answer is yes. [Ibid., emphasis in the original]

The article cited the work of Koopman and von Neumann from the 1930s, but, again, did not cite any of the other authors discussed in previous sections of the present work.

2.8 Danilo Mauro

On May 23, 2001, a preprint appeared on the arXiv, titled “On Koopman-von Neumann Waves” and authored by Danilo Mauro. The paper was later published in the *International Journal of Modern Physics* in 2002 (Mauro 2002). The paper’s opening statements were consistent with the research literature:

In their standard formulation classical and quantum mechanics are written in two completely different mathematical languages: for example in classical mechanics observables are *functions* of a $2n$ -dimensional phase space, while in quantum mechanics they are self-adjoint *operators* acting on an [sic] Hilbert space. In the literature there are

a lot of attempts to reformulate classical and quantum mechanics in similar forms. In this paper we shall concentrate on the work of Koopman and von Neumann (KvN) who proposed, in 1931-32, an operatorial formulation of classical mechanics. [Ibid., p. 1, emphasis in the original]

The statements that immediately followed, however, were historically inaccurate, because they asserted that Koopman and von Neumann began their approach by introducing classical wave functions:

The starting point of their work is the possibility of defining an [sic] Hilbert space of *complex* and *square integrable* classical “wave” functions $\psi(\varphi)$ such that $\rho(\varphi) \equiv |\psi(\varphi)|^2$ can be interpreted as a probability density of finding a particle at the point $\varphi = (q, p)$ of the phase space. This ρ has to evolve in time according to the well-known Liouville equation:

$$i \frac{\partial}{\partial t} \rho(q, p) = \hat{\mathcal{H}} \rho(q, p) \quad [\text{Mauro's eq. (1.1)}] \quad (25)$$

where $\hat{\mathcal{H}}$ is the Liouville operator $\hat{\mathcal{H}} = -i\partial_p H \partial_q + i\partial_q H \partial_p$ and H is the Hamiltonian of the standard phase space. In order to obtain (1.1) Koopman and von Neumann postulated the same evolution for ψ :

$$i \frac{\partial}{\partial t} \psi(q, p) = \hat{\mathcal{H}} \psi(q, p) \quad [\text{Mauro's eq. (1.2)}] \quad (26)$$

[Ibid., p. 1, emphasis in the original]

Notice, furthermore, that although the formula for the Liouville operator $\hat{\mathcal{H}}$ appearing in (25) was in agreement with the usual definition (5), the evolution equation (26) for ψ was off by a crucial minus sign as compared with the equation (6) satisfied by Koopman's phase-space functions.

Later, after reviewing the equations for time evolution in textbook quantum mechanics, the paper continued as follows:

The situation is completely different in the Hilbert space of classical mechanics. In fact, following Koopman and von Neumann, we postulate that the wave functions $\psi(\varphi, t) = \psi(q, p, t)$ evolve in time with the Liouvillian operator:

$$\hat{\mathcal{H}} = -i\partial_{p_i} H \partial_{q_i} + i\partial_{q_i} H \partial_{p_i} \quad [\text{Mauro's eq. (2.5)}] \quad (27)$$

according to the following equation:

$$i \frac{\partial}{\partial t} \psi = \hat{\mathcal{H}} \psi \quad \Rightarrow \quad \frac{\partial}{\partial t} \psi = (-\partial_{p_i} H \partial_{q_i} + \partial_{q_i} H \partial_{p_i}) \psi \quad [\text{Mauro's eq. (2.6)}] \quad (28)$$

We can think of (2.6) as the analogue of the quantum Schrödinger equation, i.e. as the fundamental equation governing the evolution of the vectors in the Hilbert space of classical mechanics. These vectors are the complex wave functions on the phase space obeying the normalizability condition $\int dq dp \psi^*(q, p) \psi(q, p) = 1$. [Ibid., p. 3]

As the present work has established, Koopman and von Neumann did not introduce classical wave functions, nor did they postulate that any such classical wave functions evolved according to the Liouville equation. These ideas were, in fact, originally due to Schönberg, and then developed, in some cases independently, by other researchers, including Loinger, Della Riccia, Wiener, and Sudarshan. As such, this method of classical wave functions should not properly be called “Koopman-von Neumann classical mechanics.”

This incorrect history showed up again in a preprint authored by Mauro and Gozzi that appeared on the arXiv on the same day—May 23, 2001. The preprint was titled “Minimal Coupling in Koopman-von Neumann Theory,” and was published in *Annals of Physics* in 2002 (Gozzi, Mauro 2002). The opening remarks began with:

In 1931, Koopman and von Neumann (KvN) *postulated* the same evolution equation for complex distributions $\psi(q, p)$ making up an L^2 Hilbert space:

$$\partial_t \psi(q, p) = -\hat{L}\psi(q, p) \quad [\text{Gozzi and Mauro's eq. (1.2)}]. \quad (29)$$

If we postulate [this equation] for $\psi(q, p)$, then it is easy to prove that functions ρ of the form

$$\rho = |\psi|^2 \quad [\text{Gozzi and Mauro's eq. (1.3)}] \quad (30)$$

evolve with the same equation as ψ . This is so because the operator \hat{L} contains only first [sic] order derivatives. This is not what happens in quantum mechanics (QM) where the evolution of the $\psi(q)$ is via the Schrödinger operator \hat{H} while that of the associated $\rho = |\psi|^2$ is via a totally different operator. The reason is that the Schrödinger operator \hat{H} , differently than [sic] the Liouville operator \hat{L} , contains second order derivatives. [Ibid., pp. 152–153, emphasis in the original]

An equation resembling (29) does appear in Koopman’s 1931 paper, though it is intended for describing the time evolution of observables in a classical phase space. The next statement in the 2002 paper is also historically incorrect:

By postulating the relations (1.3) and (1.2) for the ψ , KvN managed to build an operatorial formulation for classical mechanics (CM) equipped with a Hilbert space structure and producing the same results as the Liouville formulation. [Ibid.]

Koopman and von Neumann did not postulate either of Gozzi and Mauro’s equations (1.2) or (1.3). As with Mauro’s previous paper, the 2002 paper cites Koopman and von Neumann, but does not cite Schönberg or any of the other developers of the method of classical wave functions.

Soon after, Deotto, Gozzi, and Mauro collaborated on another paper, which appeared on the arXiv on August 7, 2002. The paper, titled “Hilbert Space Structures in Classical Mechanics. I,” was published in the *Journal of Mathematical Physics* in 2003 (Deotto, Gozzi, Mauro 2003). The paper began with the following statements:

In the 1930s Koopman and von Neumann (KvN) gave an operatorial formulation of *classical mechanics* (CM). They first introduced square-integrable functions $\psi(\varphi^a)$ on the phase space \mathcal{M} of a classical system with Hamiltonian $H(\varphi)$ (with φ^a we indicate the $2n$ phase-space coordinates of the system $\varphi^a = q^1 \cdots q^n, p^1 \cdots p^n$). According to KvN the Liouville phase-space distributions are obtained from $\psi(\varphi)$ as

$$\rho(\varphi) = |\psi(\varphi)|^2 \quad [\text{Deotto, Gozzi, and Mauro's eq. (1.1)}]. \quad (31)$$

The introduction of the $\psi(\varphi)$ is an acceptable assumption considering that $\rho(\varphi)$, having the meaning of a probability density, is always positive semidefinite $\rho(\varphi) \geq 0$, and so one can always take its “square root” and obtain $\psi(\varphi)$. Moreover, as $\psi(\varphi)$ is square integrable, i.e., $\psi(\varphi) \in L^2$, it turns out that $\rho(\varphi)$ is integrable as it should be

$$\int d^{2n}\varphi \psi^*(\varphi)\psi(\varphi) = \int d^{2n}\varphi \rho(\varphi) < \infty \quad [\text{Deotto, Gozzi, and Mauro's eq. (1.2)}]. \quad (32)$$

KvN *postulated* the following evolution for $\psi(\varphi)$:

$$i \frac{\partial \psi(\varphi, t)}{\partial t} = \hat{L} \psi(\varphi, t) \quad [\text{Deotto, Gozzi, and Mauro's eq. (1.3)}] \quad (33)$$

where \hat{L} , defined as

$$\hat{L} = i \frac{\partial H}{\partial q^i} \frac{\partial}{\partial p^i} - i \frac{\partial H}{\partial p^i} \frac{\partial}{\partial q^i} \quad [\text{Deotto, Gozzi, and Mauro's eq. (1.4)}] \quad (34)$$

is the Liouville operator. This equation of motion for $\psi(\varphi)$ and (1.1) lead to the same evolution for $\rho(\varphi)$,

$$i \frac{\partial \rho(\varphi, t)}{\partial t} = \hat{L} \rho(\varphi, t) \quad [\text{Deotto, Gozzi, and Mauro's eq. (1.5)}]. \quad (35)$$

This is the well-known Liouville equation satisfied by the classical probability densities. Note that $\rho(\varphi)$ obeys the same equation as $\psi(\varphi)$ because \hat{L} is first order in the derivatives. The same does not happen in quantum mechanics where the analog of (1.3) is the Schrödinger equation whose evolution operator is second order in the derivatives. We will not spend more time here in explaining the interplay between the quantum mechanical wave functions $\psi(q)$ and these “KvN waves” $\psi(\varphi)$. The interested reader can consult Ref. 2 [which refers to the two 2002 papers cited above] where many details have been worked out. [Ibid., pp. 5902–5903, emphasis in the original]

Again, the paper attributed the introduction of classical wave functions, related to classical probability distributions by the modulus-squaring operation, and the introduction of a time-evolution equation for classical wave functions, to Koopman and von Neumann.

Mauro's PhD thesis appeared on the arXiv on January 30, 2003, and was titled “Topics in

Koopman-von Neumann Theory” (Mauro 2003). The introduction, in describing attempts to connect the formalism of classical mechanics with the formalism of quantum mechanics, contained this text:

Another, even older, direction is to reformulate CM in an operatorial language by using a Hilbert space of square integrable functions on the phase space and by replacing the Poisson brackets with some suitable classical commutators. This is what has been done in the 30’s by Koopman and von Neumann (KvN). [Ibid., p. 1]

These statements were consistent with the historical record. However, a few sentences later, one finds:

The starting point of KvN is the introduction of a Hilbert space of square integrable and complex functions $\psi(q, p)$ whose modulus square are just the usual probability densities in phase space $\rho(q, p) = |\psi(q, p)|^2$. [Ibid., p. 1]

Shortly thereafter, the paper stated:

In fact KvN postulated that the evolution of the $\psi(\varphi)$ must be given by the Liouvillian which, containing only first order derivatives, evolves also the probability densities $\rho(\varphi)$, differently than [sic] what happens in QM. [Ibid., pp. 1–2]

As the present work has shown, these last two statements were not in keeping with the historical record. Similar statements showed up elsewhere in the thesis, in which $\psi(\varphi)$ was called the “KvN wave” and its Liouville equation was called the “KvN equation.” Although the thesis did not cite most of the researchers discussed in the present work, the thesis did cite Sherry and Sudarshan’s 1978 paper (Sherry, Sudarshan 1978), albeit without crediting the use of classical wave functions to Sudarshan.

The introduction to Mauro’s 2003 paper “A New Quantization Map” (Mauro 2003) contained this text:

KvN formulated classical mechanics in a Hilbert space made up of complex square integrable functions over the phase space variables $\psi(q, p, t)$. In particular they postulated, as equation of evolution for $\psi(q, p, t)$, the Liouville equation itself

$$i \frac{\partial}{\partial t} \psi(q, p, t) = \hat{L} \psi(q, p, t) \quad [\text{Mauro’s eq. (3)}]. \quad (36)$$

Starting from (3) it is easy to prove that, since the Liouvillian \hat{L} contains only first order derivatives, the Liouville equation (1) for the probability densities $\rho(q, p, t)$ can be derived via the postulate $\rho(q, p, t) = |\psi(q, p, t)|^2$. Finally KvN imposed on the states of their Hilbert space the following scalar product:

$$\langle \psi | \tau \rangle = \int dq dp \psi^*(q, p) \tau(q, p) \quad [\text{Mauro’s eq. (4)}]. \quad (37)$$

With this choice the Liouvillian \hat{L} is a Hermitian operator. Therefore $\langle\psi|\psi\rangle = \int dq dp |\psi(q, p)|^2$ is a conserved quantity and $|\psi(q, p)|^2$ can be consistently interpreted as the probability density of finding a particle in a point of the phase space. [Ibid., p. 28]

Despite the incorrect claim that Koopman and von Neumann postulated the specific equation (36), notice the careful language in these introductory statements, which otherwise said only that Koopman and von Neumann identified $\psi(q, p, t)$ as “complex square integral functions over the phase space variables” with a specific scalar product, and did not claim that Koopman or von Neumann themselves interpreted $\psi(q, p, t)$ as a classical wave function. In the quoted text above, the paper switched to the passive voice in assigning this interpretation to $\psi(q, p, t)$, both in the sentence immediately following (36), and in the last sentence of the quoted text. The scalar product appearing in (37), however, was missing the phase-space probability density $\rho(q, p)$ that appeared in the inner product (1) as defined in Koopman’s 1931 paper, and that also appeared in the integral measures used both in Koopman’s 1931 paper and in von Neumann’s two 1932 papers.

Similar statements showed up in a 2004 paper co-authored by Gozzi and Mauro, titled “On Koopman-von Neumann Waves II” (Gozzi, Mauro 2004). In the abstract, the authors wrote:

In particular we show that the introduction of the KvN Hilbert space of complex and square integrable “wave functions” requires an enlargement of the set of the observables of ordinary classical mechanics. [Ibid.]

The introduction included:

In a previous paper we stressed that KvN did not use the space of the ρ but introduced instead a Hilbert space made up of complex *square integrable* functions $\psi(q, p) \in L^2$ over phase space. These ψ are “the KvN waves” we indicated in the title. Next they *postulated* for every $\psi(q, p, t)$ an equation of evolution which is the Liouville equation itself:

$$i \frac{\partial}{\partial t} \psi(q, p, t) = \hat{\mathcal{H}} \psi(q, p, t) \quad [\text{Gozzi and Mauro’s eq. (1.3)}]. \quad (38)$$

Because the Liouvillian $\hat{\mathcal{H}}$ contains only first order derivatives, it is easy to prove that the Liouville equation (1.1) for the probability densities $\rho(q, p, t)$ can be derived from (1.3) by postulating that $\rho(q, p, t) = |\psi(q, p, t)|^2$. [Ibid., emphasis in the original]

Although the paper did not attribute the modulus-squaring relationship to Koopman and von Neumann, it did refer to ψ as a “KvN wave” and said that Koopman and von Neumann postulated its time-evolution equation.

3 Conclusion

The present paper was intended to clarify the history behind the formulation of classical mechanics developed by Bernard Koopman and John von Neumann, and to show that the method of “classical” wave functions was due not to Koopman and von Neumann, but perhaps first due to Mario

Schönberg, with later contributions from Alfred Loinger, Giacomo Della Riccia, Norbert Wiener, and E.C. George Sudarshan. Of course, even this historical assessment may be incorrect, and other researchers may have come up with the idea before Schönberg.

The method of classical wave functions has proved to be important and highly useful, and this historical misattribution should not be taken to suggest otherwise. However, getting the history right matters, especially when those responsible for an influential idea would otherwise not be given the credit that they deserve.

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