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LETTER TO THE EDITOR

Quantum mechanics as an approximation to classical mechanics in Hilbert space

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Abstract
Classical mechanics is formulated in complex Hilbert space with the introduction of a commutative product of operators, an antisymmetric bracket and a quasidensity operator that is not positive definite. These are analogues of the star product, the Moyal bracket, and the Wigner function in the phase space formulation of quantum mechanics. Quantum mechanics is then viewed as a limiting form of classical mechanics, as Planck's constant approaches zero, rather than the other way around. The forms of semiquantum approximations to classical mechanics, analogous to semiclassical approximations to quantum mechanics, are indicated.

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While our understanding of the relation between quantum mechanics and classical mechanics has steadily increased over the past 75 years, as a result of many studies from various points of view (see [1–7] and references therein), few would claim that it is complete. Meanwhile, increasing attention has focused on the interface between the quantum and classical domains, because of advances in experimental science and engineering, and the associated development of 'nanotechnology'.

Classical mechanics is usually formulated in real, finite-dimensional phase space, and quantum mechanics is usually formulated in complex, infinite-dimensional Hilbert space. However, a completely equivalent formulation of quantum mechanics in phase space is known [8–15], with a quasidistribution function that is not positive definite, in terms of which quantum mechanics is seen as a deformation of classical mechanics [14]. The phase space formulation of quantum mechanics provides a natural setting for the formulation of semiclassical approximations to quantum mechanics [1, 4, 10], which allow us to explore the interface between the two forms of mechanics when approached from the classical side.

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In his remarkable paper in 1946, Groenewold [11] indicated the alternative possibility of formulating classical mechanics as a quantum-like theory, with a quasidensity operator that is not positive definite, although few details were given. This idea has since been commented upon [14] and explored [16], notably by Muga *et al* [17]. It is not to be confused with the approach to classical mechanics in the real Hilbert space of square-integrable phase space functions [18]. Here we show that just as quantum mechanics can be formulated in phase space, so also classical mechanics can be formulated in complex Hilbert space, in such a way that quantum mechanics is seen as a limiting form of classical mechanics, emerging as Planck's constant approaches zero, rather than the other way around. And now there arises the possibility of exploring the interface between quantum mechanics and classical mechanics from the other side, the quantum side, with the development of semiquantum approximations to classical mechanics.

We limit our discussion to a system with one linear degree of freedom. All formulae below can be generalized to many (possibly infinitely many!) degrees of freedom. Our presentation is formal and heuristic; there is no attempt at mathematical rigour.

A conservative classical system is usually described in terms of functions (classical observables) $A_C(q, p)$ on phase space, together with a probability density $\rho_C(q, p, t)$, characterizing the state of the system at time t, with evolution equation

$$\begin{aligned} \frac{\partial \rho_C}{\partial t} &= \{H_C, \rho_C\}_P \equiv H_C J \rho_C \\ J &= \frac{\partial^L}{\partial q}\frac{\partial^R}{\partial p} - \frac{\partial^L}{\partial p}\frac{\partial^R}{\partial q}. \end{aligned} \tag{1}$$

Here H_C is the Hamiltonian function, $\{A, B\}_P$ denotes the Poisson bracket, and the superscripts L and R indicate the directions in which the differential operators act. The expectation value of the classical observable $A_C(q, p)$ at time t is

$$\langle A_C\rangle(t) = \int A_C(q, p)\rho_C(q, p, t)\,\mathrm{d}q\,\mathrm{d}p. \tag{2}$$

In (2) and below, integrals are over all real values of the variables of integration.

A conservative quantum system is usually described in terms of a complex Hilbert space of square-integrable state functions $\psi(x)$. Quantum observables are linear operators $\hat{A}_Q$ acting on state functions as

$$(\hat{A}_Q\psi)(x) = \int A_{QK}(x, y)\psi(y)\,\mathrm{d}y \tag{3}$$

where $A_{QK}(x, y)$ is a complex-valued function, the kernel of $\hat{A}_Q$. In particular, the canonical coordinate and momentum operators $\hat{q}$ and $\hat{p}$ have kernels $x\delta(x - y)$ and $-\mathrm{i}\hbar\delta'(x - y)$, respectively, where $\delta(x)$ is Dirac's 'delta function'. If the observable quantity is real, the corresponding operator is Hermitian: $A_{QK}(x, y) = A_{QK}(y, x)^*$. An important example is the quantum density operator $\hat{\rho}_Q(t)$, which has a kernel

$$\rho_{QK}(x, y, t) = \sum_r p_r\psi_r(x, t)\psi_r(y, t)^* \tag{4}$$

when the system is in a state described by the 'mixture' of orthogonal and normalized state functions $\psi_r(x, t)$ with associated probabilities p_r at time t. The quantum density operator is positive definite, with unit trace, and the expectation value of the quantum observable $\hat{A}_Q$ at time t is

$$\langle\hat{A}_Q\rangle(t) = \mathrm{Tr}(\hat{A}_Q\hat{\rho}_Q(t)). \tag{5}$$

The evolution equation for $\hat{\rho}_Q(t)$ is

$$\frac{\partial \hat{\rho}_Q}{\partial t} = \frac{1}{\mathrm{i}\hbar}[\hat{H}_Q, \hat{\rho}_Q] \tag{6}$$

where $\hat{H}_Q$ is the Hamiltonian operator, and $[\hat{A}_Q, \hat{B}_Q]$ denotes the commutator.

In order to map the Hilbert space formulation of quantum mechanics into the phase space formulation, the Weyl–Wigner transform $\mathcal{W}$ is introduced. For each quantum observable $\hat{A}_Q$ with kernel $A_{QK}(x, y)$, a corresponding function $A_Q = \mathcal{W}(\hat{A}_Q)$ on phase space is defined by setting

$$A_Q(q, p) = \int A_{QK}(q - x/2, q + x/2)\, \mathrm{e}^{\mathrm{i}px/\hbar}\, \mathrm{d}x. \tag{7}$$

If $\hat{A}_Q$ is Hermitian, then A_Q is real. The Wigner density function $\rho_Q(t) = \mathcal{W}(\hat{\rho}_Q(t))/(2\pi\hbar)$ is a particular case, in terms of which the quantum expectation value (5) can be rewritten as

$$\langle \hat{A}_Q \rangle(t) = \int_\Gamma A_Q(q, p)\rho_Q(q, p, t)\, \mathrm{d}q\, \mathrm{d}p. \tag{8}$$

This has the appearance of the classical average (2), but while the Wigner function is real and normalized, it is not in general non-negative everywhere on phase space, and consequently can be interpreted only as a quasiprobability density.

In order to describe dynamics in the phase space formulation, the celebrated star product and star (or Moyal) bracket of quantum phase space functions are introduced [9, 11, 12]:

$$\begin{aligned}(A_Q \star B_Q) &= \mathcal{W}(\hat{A}_Q \hat{B}_Q)\\ \{A_Q, B_Q\}_\star &= \frac{1}{\mathrm{i}\hbar}\mathcal{W}([\hat{A}_Q, \hat{B}_Q])\\ &= \frac{1}{\mathrm{i}\hbar}(A_Q \star B_Q - B_Q \star A_Q).\end{aligned} \tag{9}$$

Then $q \star p = qp + \mathrm{i}\hbar/2$, $p \star q = qp - \mathrm{i}\hbar/2$, $q^2 \star p^3 = q^2p^3 + 3\mathrm{i}\hbar qp^2 - 3\hbar^2 p$, etc. The quantum evolution (6) is now replaced by

$$\frac{\partial \rho_Q(t)}{\partial t} = \{H_Q, \rho_Q\}_\star \tag{10}$$

where $H_Q = \mathcal{W}(\hat{H}_Q)$.

For suitably smooth A_Q and B_Q, in particular polynomials in q and p, it can be shown from (9) that

$$\{A_Q, B_Q\}_\star = A_Q G B_Q \qquad G = \frac{2}{\hbar}\sin\left[\frac{\hbar}{2}J\right] \tag{11}$$

where the sine function is to be interpreted by its Taylor series, and J is as in (1). For more general A_Q, B_Q, such an expansion has only an asymptotic meaning, so that (10) leads to

$$\frac{\partial \rho_Q(t)}{\partial t} \sim H_Q J \rho_Q - \frac{\hbar^2}{3!2^2} H_Q J^3 \rho_Q + \frac{\hbar^4}{5!2^4} H_Q J^5 \rho_Q \cdots \qquad (\hbar \to 0). \tag{12}$$

Equations (8) and (12) are to be compared with their classical counterparts (2) and (1), which are 'obtained' from (8) and (12) as $\hbar$ approaches 0. It is not our purpose here to discuss the subtle mathematical difficulties associated with this limiting process [1, 4]. It suffices to say that (8) and (12) form a natural starting point for discussions of the classical limit, and of semiclassical approximations to quantum mechanics [4] as $\hbar$ approaches 0.

We now stand the foregoing phase space reformulation of quantum mechanics on its head, and instead reformulate classical mechanics in Hilbert space. With each classical phase space function $A_C(q, p)$, we associate a linear operator $\hat{A}_C = \mathcal{W}^{-1}(A_C)$. This defines $\hat{A}_C$ as the operator with kernel

$$A_{CK}(x, y) = \frac{1}{2\pi\hbar} \int A_C([x+y]/2, p)\, \mathrm{e}^{\mathrm{i}p(x-y)/\hbar}\, \mathrm{d}p. \tag{13}$$

If A_C is real, then $\hat{A}_C$ is Hermitian. This is the usual Weyl mapping [8] from functions to operators, but our intention here is not to quantize, but to reformulate classical mechanics in Hilbert space. It may then be objected that Planck's constant is not available to us in a classical theory. We treat $\hbar$ for the moment as a parameter with dimensions of action, whose value is to be specified at our convenience.

As a special case, we have the Groenewold density operator [11]

$$\hat{\rho}_C(t) = 2\pi\hbar \mathcal{W}^{-1}(\rho_C(q, p, t)). \tag{14}$$

This can be seen to be bounded, with unit trace, but unlike a true quantum density operator, it is not always positive definite. Just as the Wigner function $\rho_Q(q, p, t)$ is only a quasiprobability density, so also the Groenewold operator $\hat{\rho}_C(t)$ is only a quasidensity operator [11]. But just as quantum averages can be calculated using the Wigner function in the 'classical' formula (8), so also classical averages can be calculated using $\hat{\rho}_C(t)$ in the 'quantum' formula

$$\langle A_C \rangle(t) = \mathrm{Tr}(\hat{A}_C \hat{\rho}_C(t)) \tag{15}$$

where $\hat{A}_C$ is the operator corresponding to the classical function $A_C(q, p)$.

In order to describe classical dynamics in Hilbert space, we first introduce a distributive, associative and commutative 'odot' product of operators,

$$\hat{A}_C \odot \hat{B}_C = \mathcal{W}^{-1}(A_C B_C) = \hat{B}_C \odot \hat{A}_C. \tag{16}$$

Then for example, $\hat{q} \odot \hat{p} = \hat{p} \odot \hat{q} = (\hat{q}\hat{p} + \hat{p}\hat{q})/2$, $\hat{q}^2 \odot \hat{p}^3 = \hat{p}^3 \odot \hat{q}^2 = (\hat{q}^2\hat{p}^3 + 2\hat{q}\hat{p}^3\hat{q} + \hat{p}^3\hat{q}^2)/4$, etc. More generally, $\{\hat{q}^k \hat{p}^l\} \odot \{\hat{q}^m \hat{p}^n\} = \{\hat{q}^{k+m} \hat{p}^{l+n}\}$, where $\{\hat{q}^r \hat{p}^s\}$ denotes the Weyl-ordered operator [8, 13] corresponding to the classical monomial $q^r p^s$. This follows from (16) because $\{\hat{q}^r \hat{p}^s\} = \mathcal{W}^{-1}(q^r p^s)$.

Most generally, it can be seen from (13) that the kernels of the operators $\hat{A}_C$, $\hat{B}_C$ and $\hat{A}_C \odot \hat{B}_C$ are related by

$$\begin{aligned}(\hat{A}_C \odot \hat{B}_C)_K(x, y) = (\hat{B}_C \odot \hat{A}_C)_K(x, y) = \int A_{CK}([3x + y - 2u]/4, [x + 3y + 2u]/4) \\ \times B_{CK}([3x + y + 2u]/4, [x + 3y - 2u]/4)\, \mathrm{d}u.\end{aligned} \tag{17}$$

It is helpful to introduce the notation

$$\begin{aligned} A_q &= \partial A/\partial q \qquad A_{qp} = \partial^2 A/\partial q \partial p, \ldots \\ \hat{A}_q &= \frac{1}{\mathrm{i}\hbar}[\hat{A}, \hat{p}] \qquad \hat{A}_{qp} = \left(\frac{1}{\mathrm{i}\hbar}\right)^2 [\hat{q}, [\hat{A}, \hat{p}]], \ldots \end{aligned} \tag{18}$$

and to note that, because $A_{qp} = qG(AGp)$, etc., and

$$\mathcal{W}^{-1}(AGB) = \frac{1}{\mathrm{i}\hbar}[\hat{A}, \hat{B}] \tag{19}$$

we have $\mathcal{W}^{-1}(A_{qp}) = \hat{A}_{qp}$, etc. In (18), $\hat{q}$ and $\hat{p}$ are the usual canonical operators, except with commutator involving the parameter $\hbar$, whose value has not yet been fixed.

To describe classical dynamics, we need to introduce a new bracket, equal except for a convenient factor to the image of the Poisson bracket under the inverse Weyl–Wigner transform. We set

$$\begin{aligned}[\hat{A}_C, \hat{B}_C]_\odot &= \mathrm{i}\hbar \mathcal{W}^{-1}(\{A_C, B_C\}_P) \\ &= \mathrm{i}\hbar\big(\hat{A}_{Cq} \odot \hat{B}_{Cp} - \hat{A}_{Cp} \odot \hat{B}_{Cq}\big).\end{aligned} \tag{20}$$

Now the classical evolution equation (1) is replaced by

$$\frac{\partial \hat{\rho}_C}{\partial t} = \frac{1}{\mathrm{i}\hbar}[\hat{H}_C, \hat{\rho}_C]_\odot. \tag{21}$$

We emphasize that this formulation of classical mechanics in terms of linear operators on complex Hilbert space, incorporating the arbitrary parameter $\hbar$, and with key equations (15) and (21), is entirely equivalent to the usual phase space formulation. We can switch between corresponding points in the two descriptions with the help of the Weyl–Wigner transform $\mathcal{W}$ and its inverse $\mathcal{W}^{-1}$.

Next, we expand the odot bracket, corresponding to the expansion (11). Noting that

$$\theta = \sin\theta(1 + \theta^2/6 + 7\theta^4/360 - \cdots) \qquad |\theta| < \pi \tag{22}$$

we write

$$\begin{aligned} AJB &= AGB + \frac{1}{6}\left(\frac{\hbar}{2}\right)^2 AJ^2GB + \frac{7}{360}\left(\frac{\hbar}{2}\right)^4 AJ^4GB - \cdots \\ &= AGB + \frac{1}{6}\left(\frac{\hbar}{2}\right)^2 (A_{qq}GB_{pp} - 2A_{qp}GB_{qp} + A_{pp}GB_{qq}) + \cdots \end{aligned} \tag{23}$$

and then, applying $\mathcal{W}^{-1}$ to both sides,

$$[\hat{A}, \hat{B}]_\odot = [\hat{A}, \hat{B}] + \frac{1}{6}\left(\frac{\hbar}{2}\right)^2 ([\hat{A}_{qq}, \hat{B}_{pp}] - 2[\hat{A}_{qp}, \hat{B}_{qp}] + [\hat{A}_{pp}, \hat{B}_{qq}]) + \cdots. \tag{24}$$

The series (23) and (24) terminate if at least one of A and B is a polynomial in q and p. For more general A and B, we may expect that the series have well-defined meanings as asymptotic expansions when $\hbar \to 0$.

The classical evolution (1) then takes the form

$$\begin{aligned} \frac{\partial \hat{\rho}_C}{\partial t} \sim \frac{1}{\mathrm{i}\hbar}[\hat{H}_C, \hat{\rho}_C] - \frac{\mathrm{i}\hbar}{24}([\hat{H}_{Cqq}, \hat{\rho}_{Cpp}] - 2[\hat{H}_{Cqp}, \hat{\rho}_{Cqp}] \\ + [\hat{H}_{Cpp}, \hat{\rho}_{Cqq}]) - \cdots \qquad (\hbar \to 0). \end{aligned} \tag{25}$$

If H_C is a polynomial in q and p, then this series terminates and the asymptotic result becomes exact.

If $H_C = H(q, p) = p^2/(2m) + V(q)$, then (25) reduces to

$$\begin{aligned} \frac{\partial \hat{\rho}_C}{\partial t} \sim \frac{1}{\mathrm{i}\hbar}[H(\hat{q}, \hat{p}), \hat{\rho}_C] - \frac{\mathrm{i}\hbar}{24}[V''(\hat{q}), \hat{\rho}_{Cpp}] \\ - \frac{7\mathrm{i}\hbar^3}{5760}[V^{(iv)}(\hat{q}), \hat{\rho}_{Cpppp}] + \cdots \qquad (\hbar \to 0) \end{aligned} \tag{26}$$

which is an analogue of Wigner's equation for the evolution of his density function [10].

If we *now* identify $\hbar$ with Planck's constant, we see that equations (5) and (6) of quantum mechanics emerge formally from (15) and (25) as $\hbar$ approaches 0, so that in this sense quantum mechanics can be regarded as a limiting form of classical mechanics. Most interesting is that (15) and (25) may be expected to form a suitable starting point for semiquantum approximations to classical mechanics, analogous to semiclassical approximations to quantum mechanics.

These results may seem paradoxical. We have introduced $\hbar$ into a reformulation of classical mechanics, without affecting its predictions in any way, and see that as this parameter approaches 0, the equations of quantum mechanics emerge. Usually we say, speaking loosely, that classical mechanics is obtained from quantum mechanics as $\hbar$ approaches 0. Viewing things from the perspective provided by the above results, we argue that it is more appropriate to say that classical mechanics and quantum mechanics become asymptotically equivalent as $\hbar$ approaches 0: the interface can be approached from either side.

We conclude with a few remarks about interesting issues suggested by the preceding discussion.

(1) In quantum mechanics, the fundamental importance of the spectra of self-adjoint operators, the superposability of state functions and the nonunitary change in the density operator following a measurement is obscured in the phase space formulation. They underlie the determination of averages (8) and of initial values of Wigner functions. On the other hand, the Hilbert space formulation of classical mechanics raises the question: what is the relevance of operator spectra and the superposability of complex vectors to classical mechanics, when formulated in this way?

(2) Consider a normalized classical density at some fixed time given by

$$\rho_C(q,p) = \frac{\sqrt{\alpha\beta}}{\pi}\,\mathrm{e}^{-(\alpha q^2+\beta p^2)}. \tag{27}$$

The corresponding quasidensity operator $\hat{\rho}_C$ has kernel

$$\rho_{CK}(x,y) = \sqrt{\frac{\alpha}{\pi}}\,\mathrm{e}^{-\alpha(x+y)^2/4}\,\mathrm{e}^{-(x-y)^2/(4\beta\hbar^2)}. \tag{28}$$

It is easy to check that this operator is bounded, with unit trace, but it is not in general positive definite. If $\alpha\beta = 1/(\hbar)^2$, so that the product of the uncertainties of q and p is equal to $\hbar/2$, the kernel factorizes:

$$\rho_{CK} = \psi(x)\psi(y)^* \qquad \psi(x) = \sqrt[4]{\frac{\alpha}{\pi}}\,\mathrm{e}^{-\alpha x^2/2} \tag{29}$$

and the operator has the form of a true, positive-definite density operator, corresponding to the pure coherent state $\psi(x)$. More generally, a little thought shows that the only positive-definite quasidensity operators are those corresponding to convex linear combinations of Gaussian $\rho_C(q,p)$, each with the product of the uncertainties in q and p equal to $\hbar/2$. At the other extreme, as $\alpha \to \infty$ and $\beta \to \infty$, then $\rho_C(q,p) \to \delta(q)\delta(p)$ and $\rho_{CK}(x,y) \to 2\delta(x+y)$. This defines the starting point of a classical trajectory, as described in the Hilbert space formulation.

(3) Consider a classical system exhibiting chaos [3], for example the Henon–Heiles oscillator with two degrees of freedom and Hamiltonian

$$\begin{aligned} H_C &= H(q_1,q_2,p_1,p_2) \\ &= a\left({p_1}^2+{p_2}^2\right) + b\left({q_1}^2+{q_2}^2\right) + cq_1\left(3{q_2}^2 - {q_1}^2\right). \end{aligned} \tag{30}$$

This system is described in Hilbert space by (15) and (the obvious generalization of) (26), with the series terminating after the terms of order $\hbar$. If we choose a Gaussian initial density, generalizing (27), with arbitrarily small uncertainties in the dynamical variables then, with the help of a computer, we can in principle track the average evolution of the classical system, again with arbitrarily small uncertainties, and even if the motion is chaotic, while working in the Hilbert space formalism. This is remarkable because in the leading 'quantum approximation', obtained by neglecting the terms of order $\hbar$ in (26), the classical chaos is suppressed [1, 3].

(4) The new bracket has the 'odot derivation property' and 'odot Jacobi identity', which it inherits from the Poisson bracket:

$$\begin{aligned} &[\hat{A}, \hat{B}\odot\hat{C}]_\odot = \hat{C}\odot[\hat{A},\hat{B}]_\odot + \hat{B}\odot[\hat{A},\hat{C}]_\odot \\ &[[\hat{A},\hat{B}]_\odot,\hat{C}]_\odot + [[\hat{B},\hat{C}]_\odot,\hat{A}]_\odot + [[\hat{C},\hat{A}]_\odot,\hat{B}]_\odot = 0. \end{aligned} \tag{31}$$

Poisson algebras of phase space functions, and associated groups, should translate into interesting odot operator structures in Hilbert space.

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