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Tomita Representations of Quantum and Classical Mechanics in a Bra/Ket Formulation

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We provide a survey of the Tomita representations of quantum and classical mechanics in a language suited for physical applications, based on a modified bra/ket formalism. The mathematical structure of the abstract representation and its physical interpretation is outlined. The relation between the Dirac formulation of quantum mechanics and the present one is shown. A description is given of the classical limit of quantum mechanics. A set of concrete representations for the quantum case is provided. The formalism is applied to the free particle and the harmonic oscillator. The quantum dynamics as a perturbation on the classical dynamics is briefly considered.

1. INTRODUCTION

The bra/ket formulation of quantum mechanics provides a compact and transparent general language covering an infinitude of Hilbert space representations. Each representation is obtained from the abstract formulation by selecting a basis in the ket space, while many of the results of the theory can be obtained on the abstract level, independent of the details of the individual representation. We agree with von Neumann (1955), who stated that "Dirac... has given a representation of quantum mechanics which is scarcely to be surpassed in brevity and elegance." Its main disadvantage is its formal character, hiding mathematical intricacies, which in special cases may be of critical importance. However, in most cases it is a routine task to translate expressions in the bra/ket language into rigorously defined mathematical statements.

Nevertheless, in spite of the impressive generality of the Dirac language, it has fundamental limitations. There exist representations of quantum mechanics that are not covered by the formalism. The reason for this is that Dirac made the assumption that the representations should be irreducible,

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i.e., that the set of self-adjoint operators on the Hilbert space corresponds exactly to the set of physical quantities (observables) of the theory. Or, in group-theoretic language, that the algebra of operators of the representation is exactly the algebra generated by the symmetry group of the system (e.g., the Galilei group).

There exist, however, representations of quantum mechanics that go beyond this assumption of irreducibility. In fact, one such representation is widely used in physics, namely the representation based on Wigner functions, sometimes somewhat misleadingly called phase space functions. This formulation, originated by Wigner (1932), is reviewed by Hillery *et al.* (1984). Other representations can be obtained using techniques from the C^*-algebra formulation of quantum mechanics.

We may construct a set of representations which differs from the set covered by the Dirac formalism, and which is based on the standard von Neumann algebras of the Tomita–Takesaki theory (Takesaki, 1970). [For an introduction, see, e.g., Bratteli and Robinson (1979).] In this paper we call these representations Tomita representations. Today the use óf Tomita representations is generally limited to the select few C^*-algebra theorists. However, some of the applications clearly demonstrate the great potential of this kind of representation. The study of classical limits is one such field of application. Primas (1979) and Grelland (1985) have considered the Born–Oppenheimer approximation as a classical molecule-structure limit, using a Tomita representation. For some systems a satisfactory quantization into an ordinary irreducible representation may be difficult to achieve, as pointed out by Ford *et al.* (1990) for the case of the toral phase space. However, a quantization of the torus was actually achieved by Benatti *et al.* (1990) by using a Tomita representation. Their paper shows, moreover, how the stochastic properties may be explored, working in such a representation. Narnhofer and Thirring (1989*a*,*b*, 1990) and Hudetz (1988, 1990) have, moreover, considered precisely defined notions of quantum stochasticity in analogy with the notions of classical ergodic theory. Their results open a new area of physical investigation on specific systems. Prigogine *et al.* (1991) applied a Tomita representation in a study of the Poincaré theorem in classical and quantum mechanics.

It is also interesting to observe that the Wigner function formulation of quantum mechanics corresponds closely to one of the Tomita representations. Thus, the theory of the Tomita representations can be looked upon as a rigorous mathematical generalization of this theory. This requires, however, a modification of the Wigner formulation. The Wigner function $W(p, q)$ is obtained by the unitary Wigner transformation from the density matrix $\rho(x, y)$ in a coordinate representation. However, the density matrix is not generally a square-integrable function in the variables x, y, since it is normalized by the trace:

$$\int \rho(x, x)\, dx = 1$$

Only the density matrix of a pure state is guaranteed to be square-integrable. A mixed state is a convex linear combination of pure states. If we replace the expansion coefficients with their square roots and apply the Wigner unitary transformation to the resulting function, we obtain a Tomita representation. It turns out that much of the structure of the original Wigner theory is retained in this representation, which we consequently call the Wigner representation. The algebraic approach to the Wigner theory presented by Bohm and Hiley (1980) is closely related to the Wigner representation. The formalism of Prigogine *et al.* (1991) corresponds to a different Tomita representation, called the canonical representation in the present paper. Our square ket $|\cdot]$ replaces the double ket $|\cdot\rangle\!\rangle$ of Prigogine *et al.*

In addition to the irreducibility assumption, another important limitation of the Dirac formalism is that it does not include the special case of $\hbar = 0$—classical mechanics—although it is well known (Koopman, 1931; Reed and Simon, 1975) that classical mechanics may well be formulated in terms of Hilbert space operators. The reason is, again, the requirement that the representation should be irreducible. Classical mechanics corresponds to a commutative algebra, which does not have any irreducible operator representations. However, it has Tomita representations.

This paper has two aims. One is to provide a formulation of the theory of Tomita representations suitable for physical applications, filling some of the gap between the conventional formulations of quantum and classical mechanics and the relevant parts of the highly abstract and mathematically complex Tomita–Takesaki theory. To do this, we modify and extend the bra/ket formalism to include the Tomita representations. In order to distinguish between the two cases, we will use the square bracket $|\cdot]$ for the kets of the Tomita representations and keep the angular bracket $|\cdot\rangle$ for the usual representations considered by Dirac. By selecting different bases of the "square" ket space, we obtain a variety of new representations.

The second aim is to explore some general properties of quantum dynamics as compared to the classical case. Since the formalism in terms of square kets also includes classical mechanics, it is particularly suited for studying the quantum/classical correspondence, and it turns out to be a powerful tool for obtaining a systematic and general quantization procedure, which we call standard quantization.

Although the new class of representations still is based on Hilbert space operators, they have certain notable properties: (1) They are reducible, meaning that not all Hilbert space vectors correspond to states, and that not all self-adjoint operators correspond to physical quantities. (2) The mixed states can be represented by Hilbert space vectors, a fact which leads to a unified description of pure and mixed states. (3) The unitary operators on the generalized Hilbert space provide a nonprojective representation of the Galilei group, which simplifies the transformation expressions.

The paper is organized as follows. First we give a brief sketch of the Dirac formalism to establish the terminology. Then the square bra/ket formalism describing the Tomita representations of quantum and classical mechanics is outlined. It is shown how the process of quantization or dequantization (taking the limit $\hbar = 0$) is done in this framework. The resulting machinery is applied to some simple physical systems to see what additional insight is to be gained. It appears that the similarities and differences between quantum and classical mechanics are more clearly brought out in this kind of representation, facilitating comparison between classical and quantum dynamical systems.

2. THE DIRAC REPRESENTATION OF A GALILEAN PARTICLE

To describe the Galilean group specifically, we use a point particle moving in one dimension as a generic model. The extension to several dimensions or several particles is straightforward.

The introduction of more than one bra/ket formulation requires a precise language. The Dirac formulation covers an infinite class of concrete representations, e.g., the Schrödinger, the momentum, or the energy representation, each obtainable by the selection of a specific basis of the ket space. We therefore talk about the Dirac formalism as the abstract Dirac representation. In a similar way we will talk about the abstract Tomita representation represented by the square ket space, which will be defined below. The square ket space, too, is equipped with a variety of bases, leading to different concrete Tomita representations.

We will use capital letters, $A, B, P, Q, \ldots$, to denote operators acting on a ket space. When necessary we indicate which of the two spaces we deal with by writing $(A)_{\mathrm{D}}$ for the Dirac ket operator A and $(A)_{\mathrm{T}}$ for the square ket operator representing the same quantity. A Hilbert space vector in the Dirac representation is written $|f\rangle$. The Dirac ket space is called $\mathscr{D}$. $\mathscr{D}$ contains the Schrödinger (position) basis

$$B_{\mathrm{S}} = \{|q\rangle \mid q \in \mathbf{R}\} \tag{1}$$

The Galilean group is generated by the unitary operators of translation $U(b)$ and the operators of the Galilean boost $U(mv)$, with the properties

$$U(b)|q\rangle = |q+b\rangle \tag{2}$$

$$U(mv)|q\rangle = |q\rangle\, e^{-imvq/\hbar} \tag{3}$$

Here

$$U(b) = e^{ibP/\hbar} \tag{4}$$

$$U(mv) = e^{-imvQ/\hbar} \tag{5}$$

with the self-adjoint operators P and Q. Formally,

$$[Q, P] = i\hbar I \tag{6}$$

We also have the momentum basis

$$B_M = \{|p\rangle \mid p \in \mathbf{R}\} \tag{7}$$

$$U(b)|p\rangle = |p\rangle\, e^{ib\cdot y/\hbar} \tag{8}$$

$$U(mv)|p\rangle = |p - mv\rangle \tag{9}$$

$$\langle q|p\rangle = (2\pi\hbar)^{-1/2}\, e^{ipq/\hbar} \tag{10}$$

The Hamiltonian $H(P, Q)$ is identical to the energy operator, and the time evolution $|f\rangle_t = V(t)|f\rangle$ is generated by the time evolution operator

$$V(t) = e^{-itH/\hbar} \tag{11}$$

3. THE TOMITA REPRESENTATION

The abstract Tomita representation $(\mathscr{T}, J, P, \mathscr{A})$ consists of an abstract Hilbert space $\mathscr{T}$ of square ket vectors $|f]$, a conjugation operator J on $\mathscr{T}$, a self-dual cone P of vectors in $\mathscr{T}$, and a subalgebra $\mathscr{A}$ of operators on $\mathscr{T}$. The self-adjoint elements of $\mathscr{A}$ represent the physical quantities (observables) of the theory. In short, $\mathscr{A}$ is the *physical algebra* of the system.

The conjugation J is an antiunitary, second-order operator, i.e., it has the following properties:

$$\begin{aligned} &\text{(i)} \quad Jx|f] = x^* J|f] \quad \forall x \in \mathbf{C} \\ &\text{(ii)} \quad [g|J^*J|f] = [f|g] \\ &\text{(iii)} \quad J^2 = I \end{aligned} \tag{12}$$

P is the state cone—the normalized vectors of P represent the states of the system, including the mixed states. The property of self-duality is defined thus: $P = P^\wedge$, where $P^\wedge$ is the dual of P, i.e.,

$$P^\wedge = \{|f] \in \mathscr{T} \mid [g|f] \geq 0 \ \forall |g] \in P\} \tag{13}$$

Self-duality implies that the inner product between the vectors of P are real and positive. The cone P has the properties

$$\begin{aligned} &\text{(i)} \quad |f] \in P \Rightarrow J|f] = |f] \\ &\text{(ii)} \quad A \in \mathscr{A} \text{ and } |f] \in P \Rightarrow AJAJ|f] \in P \\ &\text{(iii)} \quad J|f] = |f] \Rightarrow |f] = |g] - |h]; \quad |g], |h] \in P \end{aligned} \tag{14}$$

The expectation value $\langle A \rangle$ of a quantity $A \in \mathscr{A}$ for the state $|f] \in P$ is

$$\langle A \rangle = [f|A|f] \tag{15}$$

To show the relation between the Dirac and the Tomita representations, we may construct the square ket space from the Dirac ket space. For this, we need an antiunitary operator T on $\mathscr{D}$. We choose T to be defined relative to the Schrödinger basis. The action of T on an arbitrary ket $|f\rangle$ is defined by

$$\langle x|(T|f\rangle) = \langle f|x\rangle \tag{16}$$

for $|x\rangle \in B_S$. We write

$$|f^*\rangle = T|f\rangle \tag{17}$$

The square ket space is now defined as $\mathscr{T} = \mathscr{D} \otimes \mathscr{D}$. From the Schrödinger basis B_S in $\mathscr{D}$ we construct *the canonical basis* B_C of $\mathscr{T}$,

$$B_C = \{|xy] = |x\rangle|y^*\rangle\} \tag{18}$$

where $|x\rangle$ and $|y\rangle$ are kets in the Schrödinger basis.

Each operator A in $\mathscr{D}$ has a counterpart in the physical algebra $\mathscr{A}$, defined by its action on a basis ket $|xy]$ by

$$(A)_T|xy] = ((A)_D|x\rangle)|y^*\rangle \tag{19}$$

or,

$$(A)_T = (A)_D \otimes (I)_D \tag{20}$$

It is easily seen that

$$J(A)_T J = (I)_D \otimes (A)_D \tag{21}$$

The physical quantity represented by $(A)_D$ acting in the Dirac ket space is represented by $(A)_T$ in the square ket space. The position and momentum operators constructed this way act as

$$Q|xy] = x|xy] \tag{22}$$

$$P|xy] = (2\pi\hbar)^{-1/2} \int e^{-isx/\hbar} s|sy]\, ds \tag{23}$$

Now we are in a position to identify the conjugation J and the self-dual cone P. The conjugation J is determined by T,

$$J|x\rangle|y\rangle = |y^*\rangle|x^*\rangle \tag{24}$$

The self-dual cone P is the set of vectors of the form

$$|f] = \sum_j |j\rangle|j^*\rangle c_j \tag{25}$$

where $\{|j\rangle\}$ is any countable, orthonormal basis for $\mathscr{D}$, and the c_j are positive reals such that $\sum_j c_j^2$ is finite.

The states are represented by normalized vectors in P. Thus, the vectors of $\mathscr{T}$ *outside* P cannot be interpreted as state vectors. We have two kinds of states: pure and mixed. The pure state corresponding to a Dirac ket $|f\rangle$ is represented by the square ket $|f]=|f\rangle|f^*\rangle$. Obviously, this is a vector in P.

A mixed state is usually described as a probability distribution $|j\rangle \to p_j$ of an orthonormal basis $\{|j\rangle\}$ in $\mathscr{D}$, for instance, represented by the density matrix $D=\sum_j |j\rangle p_j\langle j|$. In the Tomita representation this mixed state is represented by the vector

$$|f]=\sum_j (p_j)^{1/2}|j\rangle|j^*\rangle \tag{26}$$

It follows that, in fact, any vector in P can be interpreted as one particular pure or mixed state.

The inner product in the space $\mathscr{T}$ of two states is different from that of the space $\mathscr{D}$. Let $|f]$ be the state vector (26), while

$$|g]=\sum_k (p_k)^{1/2}|k\rangle|k^*\rangle \tag{27}$$

Then,

$$[g|f]=\sum_{jk} (p_j p_k)^{1/2}|\langle k|j\rangle|^2 \tag{28}$$

For pure states we obtain

$$[j|k]=|\langle j|k\rangle|^2 \tag{29}$$

The expectation value of an operator A is, for a pure state $|j]$,

$$\begin{aligned}\langle A\rangle &= [j|(A)_{\rm S}|j]\\ &=\langle j^*|\langle j|((A)_{\rm D}|j\rangle)|j^*\rangle\\ &=\langle j|(A)_{\rm D}|j\rangle\end{aligned} \tag{30}$$

and, for a mixed state $|f]=\sum_j (p_j)^{1/2}|j\rangle|j^*\rangle$,

$$\begin{aligned}\langle A\rangle &= [f|(A)_{\rm S}|f]\\ &=\sum_j\sum_k (p_j)^{1/2}(p_k)^{1/2}\langle j|(A)_{\rm D}|k\rangle\langle j^*|k^*\rangle\\ &=\sum_j p_j\langle j|(A)_{\rm D}|j\rangle\end{aligned} \tag{31}$$

We see that the usual expression for the expectation value extends to the mixed states.

Nondiagonal matrix elements $[j|A|k]$ are not related to transition probabilities, as one may have hoped. For pure states from an orthonormal set $\{|j]\}$,

$$[j|A|k] = \langle j|(A)_{\mathrm{D}}|k\rangle\langle k|j\rangle$$
$$= \langle j|(A)_{\mathrm{D}}|k\rangle\delta_{jk} \tag{32}$$

whereas for the nonpure states $|f] = \sum_j |j]b_j$ and $|g] = \sum_j |j]c_j$

$$[f|A|g] = \sum_j b_j c_j \langle j|(A)_{\mathrm{D}}|j\rangle \tag{33}$$

Thus, if $\{|j\rangle\}$, and hence also $\{|j]\}$, are orthonormal sets, the matrix of A does not have off-diagonal elements between pure state vectors.

To express transition probabilities, we need the conjugation J:

$$[f|AJAJ|g] = \langle {}^*f|\langle f|AJAJ|g\rangle|g^*\rangle$$
$$= \langle {}^*f|\langle f|AJA|g\rangle|g^*\rangle$$
$$= \langle {}^*f|\langle f|AJ((A)_{\mathrm{D}}|g\rangle)|g^*\rangle$$
$$= \langle {}^*f|(\langle f|(A)_{\mathrm{D}})|g\rangle((A)_{\mathrm{D}}|g^*\rangle)$$
$$= |\langle f|(A)_{\mathrm{D}}|g\rangle|^2 \tag{34}$$

We then consider the dynamics. The time evolution operator on the square ket space $U(t)$ is also constructed from the unitary operator $V(t) = e^{-itH/\hbar}$ by using J:

$$U(t) = V(t)JV(t)J = e^{-it(H-JHJ)/\hbar} = e^{-tL} \tag{35}$$

Property (14)(ii) ensures that $U(t)$ maps state vectors onto state vectors, i.e., that P is invariant under $U(t)$. We see that the generator of time evolution in a Tomita representation is different from the energy operator $(H)_{\mathrm{D}}$. The operator $L = i(H - JHJ)/\hbar$ is the quantum analog of the classical Liouville operator, and is called the *quantum Liouvillian.*

It is easily seen that application of $U(t)$ leads to the correct Schrödinger equation. Consider the state $|f] = |j\rangle|j^*\rangle$:

$$i\hbar(\partial/\partial t)|f] = i\hbar(\partial/\partial t)|j\rangle|j^*\rangle + i\hbar|j\rangle(\partial/\partial t)|j^*\rangle$$
$$= ((H)_{\mathrm{D}}|j\rangle)|j^*\rangle + |j\rangle(-(H)_{\mathrm{D}}|j^*\rangle)$$
$$= ((H)_{\mathrm{T}} - J(H)_{\mathrm{T}}J)|f] \tag{36}$$

4. THE GALILEI GROUP

The unitary representation of the Galilei group is constructed in a way similar to that applied in the construction of the time evolution operator.

The translation a distance b is carried out by the operator

$$U(b) = e^{-ib(P-JPJ)/\hbar} \tag{37}$$

whereas the Galilei boost with a velocity v is represented by

$$U(v) = e^{imv(Q-JQJ)/\hbar} \tag{38}$$

There exists one particular basis in the square ket space that transforms in a fashion similar to a point in the phase space of the particle. This basis relates to the Wigner functions, which correspond essentially to vectors in P represented in this nicely transforming basis. An appropriate name for the basis is therefore the Wigner basis, B_W. This basis is related to the canonical basis B_C in the following way: Let $B_W = \{|qp]\}$ and $B_C = \{|xy]\}$. Then

$$[xy|qp] = (2\pi\hbar)^{-1/2}\delta(q-(x+y)/2)\, e^{i(x-y)p/\hbar} \tag{39}$$

The action of the unitary operators of the Galilei group on the Wigner basis is

$$U(b)|qp] = |q+b, p] \tag{40}$$

$$U(v)|qp] = |q, p+mv] \tag{41}$$

Moreover,

$$U(v)\,U(t)|qp] = U(v)|qp]_t = |q+vt, p+mv]_t \tag{42}$$

Being a possible carrier of a nonprojective representation of the Galilei group is one of the major advantages of the square ket representation, and a necessary condition for the ket space to carry both the quantum and the classical algebra of point mechanics.

5. DECOMPOSITION OF THE POSITION AND MOMENTUM OPERATORS

To study the transition $\hbar \to 0$, it is useful to make a decomposition of the operators of position and momentum.

We define the generators of the Galilei group

$$D = (P-JPJ)/\hbar \tag{43}$$

and

$$E = (Q-JQJ)/\hbar \tag{44}$$

We also define the self-adjoint operators

$$Q_0 = (Q+JQJ)/2 \tag{45}$$

and

$$P_0 = (P + JPJ)/2 \tag{46}$$

with the properties

$$[Q_0, P_0] = [D, E] = [Q_0, E] = [P_0, D] = 0 \tag{47}$$

while

$$[Q_0, D] = -[P_0, E] = iI \tag{48}$$

We can now express the position and momentum operators in terms of these operators:

$$\begin{aligned} Q &= Q_0 + \hbar E/2 \\ P &= P_0 + \hbar D/2 \\ JQJ &= Q_0 - \hbar E/2 \\ JPJ &= P_0 - \hbar D/2 \end{aligned} \tag{49}$$

Here, the noncommuting coordinates Q and P are expressed as a sum of a *commuting set* of coordinates, plus correction terms, proportional to $\hbar$. Thus, we are in a nice position to consider the limit $\hbar \to 0$.

We are now able to write down the quantum Liouvillian in terms of the decomposed operators. The Liouvillian is of the form

$$\begin{aligned} -i\hbar L &= H - JHJ \\ &= (P^2 - JP^2J)/2m + V(Q) - JV(Q)J \\ &= -i\hbar L_0 - i\hbar\Delta \end{aligned} \tag{50}$$

where

$$L_0 = (i/m)P_0 D + iV'(Q_0)E \tag{51}$$

and

$$\Delta = (i/\hbar)(V(Q) - JV(Q)J) - iV'(Q_0)E \tag{52}$$

If Δ is expanded in a Taylor series about Q_0, the second term on the right-hand side of (52) cancels the first nonzero term of the Taylor expansion. Thus, Δ represents a second-order term in $\hbar$. We have $L = L_0$ for a free particle, a particle moving in a linear potential, and a harmonic oscillator.

We now want to consider an important new feature of the Tomita representation as compared to the Dirac representation: The energy operator is different from the time evolution operator. From (50), together with the fact that a ket in P is invariant under J, we infer that an eigenket of H in P is also an eigenket of L with eigenvalue 0.

The energy operator H is

$$\begin{aligned} H &= P^2/2m + V(Q) \\ &= (1/2m)P_0^2 + (h/2m)P_0 D + (h^2/8m)D^2 + V(Q_0) \\ &\quad + (h/2)V'(Q_0)E + (h^2/8)V''(Q_0)E^2 + \cdots \end{aligned} \tag{53}$$

assuming that V can be expanded in a Taylor series.

6. THE CLASSICAL LIMIT

It is easily seen that

$$\begin{aligned} Q &\to Q_0 \quad \text{as} \quad \hbar \to 0 \\ P &\to P_0 \quad \text{as} \quad \hbar \to 0 \end{aligned} \tag{54}$$

in the *strong resolvent* sense. Operator convergence $A_\hbar \to A_0$ in the strong resolvent sense means that $A_\hbar|\psi] \to A_0|\psi]$ for suitable vectors, or, equivalently, $e^{itA_\hbar}|\psi] \to e^{itA_0}|\psi]$ for all t and all vectors in $\mathscr{T}$. Thus, we see that, in a specified topological sense, the noncommuting set of quantum coordinates approaches a commutative set in the classical limit.

Classical mechanics corresponds to the case $\hbar = 0$. The physical quantities are then represented by the commutative algebra generated by Q_0 and P_0.

It is of physical relevance in *which sense* the convergence above exists, because the convergence criterion (topology) determines what properties go smoothly into the classical domain and what properties may have an abrupt change. Strong resolvent convergence implies that the spectrum cannot suddenly expand at the limit. This means that each value of the spectrum of the classical operator will have at least one value in the spectrum of its quantum correspondent that approaches it in the limit. However, the spectrum may suddenly contract, which implies sudden loss of information at the limit. To prevent contraction, one needs norm resolvent convergence, which is *not* what we have here.

Furthermore, we cannot *a priori* assume a smooth transition of the eigenvector corresponding to a spectral value at the limit $\hbar = 0$, we can only count on a smooth transition of the eigenvalue itself. Contraction at the $\hbar = 0$ limit means that a single point in the classical spectrum may dissolve into a range of values through quantization. An example is the single stationary energy value of the classical harmonic oscillator, which is mapped into the whole eigenvalue spectrum of the Hamiltonian through quantization.

The limiting process is completed by considering the time evolution at the $\hbar = 0$ limit. The quantum Liouvillian is written as the sum

$$L = L_0 + \Delta \tag{55}$$

The first term is the surviving term at the limit $\hbar = 0$, whereas the last term may be interpreted as a quantum correction term. This term may be expanded to the leading order:

$$\Delta = L_1 + O(\hbar^4) \tag{56}$$

where

$$L_1 = (i\hbar^2/24)\, V'''(Q_0)\, E^3 \tag{57}$$

Here, V''' means the third derivative of V. The expressions are obtained by a formal Taylor expansion. Note that the higher terms of L also contain correspondingly high derivatives of V. In particular, if V is a second-order polynomial (harmonic oscillator), then $L = L_0$. We call L_0 the *classical Liouvillian*, since

$$iL \to iL_0 \qquad \text{as} \quad \hbar \to 0 \tag{58}$$

in the strong resolvent sense, i.e., that

$$e^{-tL} \to e^{-tL_0} \qquad \text{as} \quad \hbar \to 0 \tag{59}$$

in the strong sense. In this way, the Tomita representation provides a nice description of the classical limit of quantum mechanics, in the sense $\hbar \to 0$.

This formalism provides a universal quantization procedure, which we will call *standard quantization.* In this quantization procedure, we start by formulating the classical system in terms of commuting (usually multiplication) operators Q_0, P_0 on the Hilbert space of phase space functions. The system is quantized by replacing these by $Q = Q_0 + \hbar E/2$ and $P = P_0 + \hbar D/2$ in the same representation.

7. THE WIGNER REPRESENTATION

To display the connection between the square ket space and the representation of quantum mechanics in terms of Wigner state functions, we will express some of the equations above in the Wigner basis (39). We define

$$f(q, p) = [qp|f] \tag{60}$$

The square-integrable function $f(q, p)$ is related to the Wigner function $W(q, p)$ as described in the introduction. In the Wigner basis the operators defined in the previous section attain the form

$$\begin{aligned} Q_0 f(q,p) &= q f(q,p) \\ P_0 f(q,p) &= p f(q,p) \\ D f(q,p) &= i(\partial/\partial q) f(q,p) \\ E f(q,p) &= -i(\partial/\partial p) f(q,p) \end{aligned} \tag{61}$$

This leads directly to the expressions for the position and momentum operators:

$$\begin{aligned} Q &= q^{\cdot} - (i\hbar/2)\partial/\partial p \\ P &= p^{\cdot} + (i\hbar/2)\partial/\partial q \end{aligned} \tag{62}$$

as well as

$$\begin{aligned} Jf(q,p) &= f^*(q,p) \\ JQJ &= q^{\cdot} + (i\hbar/2m)\,\partial/\partial p \\ JPJ &= p^{\cdot} - (i\hbar/2)\,\partial/\partial q \end{aligned} \tag{63}$$

Note that since neither the position nor the momentum operator is a multiplication operator, the corresponding state functions of the cone P are *not* probability distributions of any of these quantities. This is a *general* fact, independent of whether the functions accidentally turn out to be nonnegative. However, we note that the state functions are real, since they are invariant under J.

The energy operator (Hamiltonian) has the form

$$H(P,Q) = \tfrac{1}{2}m^{-1}(p^2 - (\hbar^2/4)(\partial^2/\partial q^2) + i\hbar p\cdot\partial/\partial q) + V(Q) \tag{64}$$

The quantum Liouvillian attains the form

$$L = m^{-1}p\cdot\partial/\partial q + V(Q) - V(JQJ) \tag{65}$$

In this basis, L_0 is the well-known classical Liouvillian

$$L_0 = m^{-1}p\cdot\partial/\partial q - V'(q)\cdot\partial/\partial p \tag{66}$$

The first quantum correction becomes

$$L_1 = -(\hbar^2/24m^3)\,V'''(q)\,\partial^3/\partial q^3 \tag{67}$$

The transformations of the Galilei group are expressed as

$$\begin{aligned} U(b)f(q,p) &= f(q-b,p) \\ U(v)f(q,p) &= f(q,p-mv) \end{aligned} \tag{68}$$

or, in the Schrödinger picture, $f_t = U(t)f$,

$$U(v)f_t(q,p) = f(q - vt, p - mv) \tag{69}$$

8. A LOCAL BASIS FOR THE *CLASSICAL* POSITION

In dealing with complicated potentials, it is useful to have a multiplicative potential operator. This can also be obtained in the Tomita representation by selecting the proper basis. We will consider two such bases, one in which the x variable is associated with the *classical* position, and one for which it is associated with the *quantum* position.

The first one, which we denote by $|uv]$, is defined relative to the Wigner basis by

$$[uv|qp] = (2\pi)^{-1/2}\, e^{ivp}\delta(u-q) \tag{70}$$

This change of basis corresponds to a Fourier transformation in the second variable. We consider state functions in the new basis,

$$f(u, v) = [uv|f] \tag{71}$$

The relevant operators become

$$\begin{aligned} Q_0 f(u, v) &= uf(u, v) \\ P_0 f(u, v) &= -i\, \partial/\partial v\, f(u, v) \\ Df(u, v) &= -i\, \partial/\partial u\, f(u, v) \\ Ef(u, v) &= vf(u, v) \end{aligned} \tag{72}$$

which lead to

$$\begin{aligned} Qf(u, v) &= (u + (\hbar/2m)v)f(u, v) \\ Pf(u, v) &= -i(\partial/\partial v + (\hbar/2)\, \partial/\partial u)f(u, v) \end{aligned} \tag{73}$$

The classical Liouvillian attains the form

$$L_0 = (i/m)(-\partial^2/\partial u\, \partial v + V'(u)v) \tag{74}$$

with the first quantum correction

$$L_1 = (i\hbar^2/24m^3)\, V'''(u)v^3 \tag{75}$$

9. A LOCAL BASIS FOR THE *QUANTUM* POSITION

The basis in which the x variable is associated with the quantum position is defined in Section 3. It is the canonical basis $\{|xy]\}$ (18). We consider

$$f(x; y) = [xy|f] \tag{76}$$

The important advantage of this representation is that if we know the Schrödinger wave function $\psi(x)$ of the state, the state function in the local representation is $f(x, y) = \psi(x)\psi(y)^*$. The relevant operators attain the form

$$\begin{aligned} Jf(x, y) &= f^*(y, x) \\ Q_0 f(x, y) &= (1/2)(x+y)f(x, y) \\ P_0 f(x, y) &= -(i\hbar/2)(\partial/\partial x - \partial/\partial y)f(x, y) \\ Df(x, y) &= -i(\partial/\partial x + \partial/\partial y)f(x, y) \\ Ef(x, y) &= \hbar^{-1}(x-y)f(x, y) \end{aligned} \tag{77}$$

which lead to

$$\begin{aligned} Qf(x, y) &= xf(x, y) \\ Pf(x, y) &= -i\hbar\, \partial/\partial x\, f(x, y) \end{aligned} \tag{78}$$

We also have that

$$\begin{aligned} JQJf(x, y) &= yf(x, y) \\ JPJf(x, y) &= i\hbar\, \partial/\partial y\, f(x, y) \end{aligned} \tag{79}$$

We obtain the following formal expression of the quantum Liouvillian:

$$L = -i\hbar(H(x) - H(y)) \tag{80}$$

Moreover

$$L_0 = (-i\hbar/2m)(\partial^2/\partial x^2 - \partial^2/\partial y^2) + (i/\hbar)\, V'((x+y)/2)(x-y) \tag{81}$$

with the first quantum correction

$$L_1 = -(1/2\hbar)\, V'''((x-y)/2)(x-y)^3 \tag{82}$$

It may come as a surprise that the constant $\hbar$ appears even in the classical case. This is due to the dual role played by $\hbar$ in using this basis. The physically relevant appearance of $\hbar$ comes from the Galilei group, and is present in the expressions relating Q, P to Q_0, P_0. However, in addition, $\hbar$ enters the unitary transformation connecting the Wigner representation and the canonical representation, and this h cannot be set equal to zero, even in the classical limit. It is one of the advantages of the abstract bra/ket formulation that these two uses of $\hbar$ can be kept separate.

The transformation relating this local representation and the Wigner representation can be obtained from (39) and expressed as operators on functions. Let $f_w(q, p)$ be the Wigner representative. The canonical representative $f_P(x, y)$ is

$$f_P = V(I \otimes U_F)f_w \tag{83}$$

where V is the coordinate transformation

$$[Vf](x, y) = f((x+y)/2, (y-x)/2)$$

and U_F is a Fourier transformation.

The energy operator of this representation is the usual Schrödinger Hamiltonian acting on the variable x. However, we can take advantage of the work we have done on the ket level, and derive the lowest order terms of expanded Hamiltonian from (53), using the expressions of (77):

$$H = H_0 + H_1 + \cdots \tag{84}$$

$$\begin{aligned} H_0 &= p_0^2/2m + V(Q_0) \\ &= -(\hbar^2/8m)(\partial^2/\partial x^2 + \partial^2/\partial y^2 - 2\,\partial^2/\partial x\,\partial y) + V((x+y)/2) \end{aligned} \tag{85}$$

$$\begin{aligned} H_1 &= (\hbar/2m)(P_0 D + V'(Q_0)E) \\ &= -(\hbar^2/4m)(\partial^2/\partial x^2 - \partial^2/\partial y^2) + V'((x+y)/2)(x-y)/2 \end{aligned} \tag{86}$$

10. CLASSICAL MECHANICS

The conventional Hilbert space formulation of classical mechanics is obtained by choosing the Wigner representation of the commutative algebra generated by P_0 and Q_0. This formulation is only a slight modification of the statistical Liouville theory, basing the description on real square-integrable amplitudes $f(q, p)$ instead of integrable probability distributions $p(q, p) = f^2(q, p)$. The reformulation in terms of square kets increases the flexibility with respect to the choice of representations.

To be able to work on the abstract ket level, we may need an operator definition of the Poisson bracket. This is provided by using the self-adjoint operators D, E defined in (43), (44). Let A, B be arbitrary operators. The *Poisson bracket* of the pair is the operator

$$\{F, G\} = [D, F][E, G] - [E, F][D, G] \tag{87}$$

When working in a representation of phase space functions, i.e., in the Wigner representation, this definition coincides with the customary one, as will be seen by substituting the explicit expressions for D and E in that representation. In particular, we note that

$$\{Q, P\} = \{Q_0, P_0\} = 1 \tag{88}$$

The physical algebra of classical mechanics is the commutative operator algebra generated by the position operator Q_0 and momentum operator P_0. The states are represented by normalized kets in a self-dual cone P_+, with the associated conjugation J, such that

$$\langle A \rangle = [f|A|f] \tag{89}$$

is the expectation value of the quantity A in the state $|f]$.

The state cone is conveniently described in the Wigner basis as the set of positive functions:

$$P_+ = \{|f]\,|\,[qp|f] \geq 0\} \tag{90}$$

The conjugation J is the same as for the quantum case, i.e., complex conjugation in the Wigner representation.

The evolution operator is the classical Liouvillian,

$$L_0 = (i/m)P_0 D + (i/m)V'(Q_0)E \qquad \text{[Eq. (51)]}$$

$$|\dot{\xi}] = -L_0|\xi] \tag{91}$$

(91) represents the equation of motion of the *Schrödinger picture of classical mechanics*, the analog of the Liouville equation. Operator analogs of Hamilton's equations, as well as Newton's second law, are obtained by working in the *Heisenberg* picture:

$$P_0(t) = U^{tL} P_0 U^{-tL} \tag{92}$$

$$\begin{aligned} P_0 &= [L, P_0] \\ &= \{H, P_0\} \\ &= -V'(Q_0) \end{aligned} \tag{93}$$

11. THE FREE PARTICLE

We now turn to the consideration of systems that have identical quantum and classical Liouville operators, and where the Heisenberg equations of motion can be solved exactly. First we will take a fresh look at the motion of a free particle.

The solutions of the Heisenberg equation are most conveniently obtained by working in the Wigner representation, where $L = y\, d/dx$, choosing $m = 1$. This leads immediately to the Schrödinger picture solution

$$f_t(x, y) = f(x - yt, y) \tag{94}$$

and to the Heisenberg picture solutions

$$\begin{aligned} Q_0(t) &= Q_0 + tP_0 \\ P_0(t) &= P_0 \\ E(t) &= E + tD \\ D(t) &= D \\ Q(t) &= Q + tP \\ P(t) &= P \end{aligned} \tag{95}$$

The *difference* between classical and quantum mechanics is reflected in the dispersion of the quantum position, even for pure states. By dispersion, we mean the increase with time of the value of $\Delta Q(t) = [\langle Q(t)^2\rangle - \langle Q(t)\rangle^2]^{1/2}$.

We are interested in the asymptotic behavior as $t \to \infty$. By inserting the Heisenberg solutions, one easily sees that

$$\Delta Q(t) \to t\,\Delta P(0) \to \infty \tag{96}$$

The origin of the dispersion is related to the initial uncertainty of P. By decomposing P, this uncertainty can be decomposed:

$$\Delta P = \Delta P_0 + \tfrac{1}{4}\hbar^2\,\Delta D + \hbar(\langle P_0 D\rangle - \langle P_0\rangle\langle D\rangle) \tag{97}$$

The first term represents the classical uncertainty. D is conjugate to Q_0, in the sense that $[Q_0, D] = i\hbar I$. Thus the next term is the uncertainty in P resulting from the uncertainty relations and the localization of Q_0. Comparing these expressions with the expression for the classical dispersion,

$$\Delta Q_0(t) \to t\,\Delta P_0(0) \to \infty \tag{98}$$

we see that the quantum dispersion is always greater than the classical one, due to the uncertainty relations.

To avoid classical dispersion, one needs a distribution sharply confined to a line $p = r$ parallel to the q axis, i.e., a state function of the form

$$f(q, p) = g(q)\delta(p - r) \tag{99}$$

The Schrödinger evolution of this state is

$$f_t(q, p) = g(q - tp)\delta(p - r) \tag{100}$$

In the special case where g is translationally invariant, i.e., a constant function, this state will be completely stationary, not because of a lack of motion of the *points* in the phase space, but because this motion does not affect the *distribution*.

The property of dynamic mixing can roughly be characterized as an asymptotic change of the distribution toward a uniform distribution of the quantities. Thus, as the variance of the quantum position increases faster than that of the classical position, a quantum system will generally be more strongly mixing than the corresponding classical system.

12. THE HARMONIC OSCILLATOR

It is well known that the similarity between classical and quantum mechanics is still strong in the case of a harmonic oscillator. This becomes obvious when working with the Tomita representations, since in this case the quantal and the classical Liouville operators are still identical. We want to explore this a bit further by introducing a new representation, based on action–angle coordinates.

The Hamiltonian of this system is

$$H = \tfrac{1}{2}(P^2 + Q^2) \tag{101}$$

deriving from the potential $V(Q) = \tfrac{1}{2}Q^2$.

Our starting point is the Wigner basis, and the transformation is a local coordinate transformation of this basis. The new basis is denoted $B_A = \{|r\theta]\}$:

$$[r\theta|f] = [2r\cos 2\pi\theta, 2r\sin 2\pi\theta|f] \tag{102}$$

where the right-hand function is the Wigner representative. The inverse transformation is

$$[xy|f] = [(x^2 + y^2)/2, \arctan(y/x)/2\pi|f] \tag{103}$$

where the right-hand function is the angle–action representative.

Here the function $f(r, \theta) = [r\theta|f]$ is defined on the half-cylinder $(0, \infty) \times [0, 1]$ subject to the periodicity condition $f(r, \theta+1) = f(r, \theta)$.

The Liouvillian attains the form

$$L = -\partial/\partial\theta \tag{104}$$

leading to the time evolution

$$U_t f(r, \theta) = f(r, \theta + t) \tag{105}$$

both in the quantum and in the classical case. Thus, the only motion possible is a periodic motion of frequency 1, both in classical and in quantum mechanics. Moreover, the stationary states are the ones that are functions of r only.

When leaving the harmonic case, we have to introduce a quantum correction into the Liouvillian. It is, however, difficult to imagine that an irregular or chaotic classical motion will be regularized by adding such terms. It is therefore of interest to ask if the apparent tendency of quantum mechanical systems to behave less irregularly than their classical correspondents is mostly a result of inappropriate methods of comparison. This will be the subject of a forthcoming paper.

The classical Hamiltonian of the harmonic oscillator is

$$H_0 f(r, \theta) = rf(r, \theta) \tag{106}$$

whereas the quantum Hamiltonian is considerably more complex:

$$H = H_0 + i\hbar L + \hbar^2(2r\, d^2/dr^2 + d^2/d\theta\, dr + (1/2r)\, d^2/d\theta^2)/4 \tag{107}$$

A *stationary state* is independent of θ (i.e., it is a uniform distribution along this coordinate) and has eigenvalue 0 with respect to L, and the restriction $H\backslash$ of H to such a state is

$$H\backslash f(r) = (r - (\hbar^2 r/2)\, d^2/dr^2) f(r) \tag{108}$$

13. THE CUBIC PERTURBATION

When the potential of the Hamiltonian includes cubic terms, we must include the perturbation $U_t = \exp(-tL_1)$. We will consider the stochastic properties of this perturbation when the potential only contains up to cubic terms, so that $(h^2/24m^3)V'''(Q_0) = k$, a constant.

U_t is mixing if

$$[qp|U_t|q'p'] \to 0 \qquad \text{as} \quad t \to \infty \tag{109}$$

(the decay property). We consider the asymptotic limit of

$$\begin{aligned}
&[qp|U_t|q'p'] \\
&\quad = \iiiint [qp|uv][uv|U_t|u'v'][u'v'|q'p']\, du\, dv\, du'\, dv' \\
&\quad = (\delta(q-q')/2\pi) \iint \exp(ivp)\exp(-iv'p')\exp(-iktv^3)\delta(v-v')\, dv\, dv' \\
&\quad = (\delta(q-q')/2\pi) \int \exp(iv(p-p'))\exp(-iktv^3)\, dv \\
&\quad \to (1/2\pi) \int \exp(-iktv^3)\, dv \\
&\quad = (1/2\pi) \int \cos(ktv^3)\, dv \\
&\quad = [\Gamma(1/3)\cos(p/6)/3k^{-1/3}]t^{-1/3} \\
&\quad \to 0 \qquad \text{as} \quad t \to \infty
\end{aligned} \tag{110}$$

We see that the matrix element (correlation function) decays to zero; thus we have the mixing property. However, it decays like $t^{-1/3}$, not exponentially fast, which is a property characteristic of chaotic systems. We can, however, conclude that the quantum perturbation contributes to the sochasticity of the system.

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