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Logical Reformulation of Quantum Mechanics. IV. Projectors in Semiclassical Physics

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This is a technical paper providing the proofs of three useful theorems playing a central role in two kinds of physical applications: an explicit logical and mathematical formulation of the interpretation of quantum mechanics and the corresponding description of irreversibility. The Appendix contains a brief mathematical introduction to microlocal analysis. Three theorems are derived in the text: (A) Associating a projector in Hilbert space with a macroscopic regular cell in classical phase space. (B) Specifying the algebra of the projectors associated with different cells. (C) Showing the connection between the classical motion of cells and the Schrödinger evolution of projectors for a class of regular Hamiltonians corresponding approximately to deterministic systems as described within the framework of quantum mechanics. Applications to the interpretation of quantum mechanics are given and the consequences for irreversibility will be given later.

KEY WORDS: Semiclassical physics; projectors; microlocal analysis.

1. INTRODUCTION

This paper belongs to a series devoted to a consistent logical interpretation of quantum mechanics.[1] It contains the proof of three theorems which allow one to derive the main features of classical physics, starting from consistent quantum representations of logic as described in I. Here classical logic enters together with classical dynamics in the definition of classical physics.

The relation between quantum dynamics and classical dynamics is an old subject.[2,3] Its best-known formulation is given by Ehrenfest's theorem,[4] which is, however, somewhat misleading since it results in

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classical equations of motion involving an average force and not the exact classical force at the average position. Decisive progress was made by Hepp,[5] who was able to recover the whole algebra of time-dependent classical position and momentum as an average of the associated operators for Gaussian wave packets, i.e., coherent wave functions.[6] Ginibre and Velo[7] have shown that this result can be extended to express classical dynamics as an asymptotic series in powers of $\hbar^{1/2}$. A form quite useful in practice has been given by Hagedorn.[8,9]

In quantum logic, propositions are expressed in terms of some projectors,[10,11] whereas classical logic, when applied to mechanics, refers to the state of the system as being in some specific cell in classical phase space, an idea going back to Poincaré. The possibility of relating these two viewpoints is contained below in Theorem A, stating essentially that one can associate some "projectors" F with a cell C in phase space. Such an operator F shares many properties of a finite-rank projector as being self-adjoint, compact, having its eigenvalues in the interval $[0, 1]$, and being such that the operator $\delta F = F^2 - F$ is small (whereas δF would exactly be zero if F were a true projector). These properties are true only when the cell C has a large volume in units $\hbar$ and a smooth enough boundary. The precise statement of the theorem is given in Section 2.

One also needs to have some control over the commutator of two approximate projectors F_1 and F_2, respectively, associated with two cells C_1 and C_2. This will be the subject of Theorem B.

When an approximate projector F or rather $F/(\mathrm{Tr}\, F)$ is treated as a state operator (i.e., a state operator ρ), its quantum dynamical evolution is given by $F(t) = U(t)\, F U^{-1}(t)$, where $U(t) = \exp(-iHt/\hbar)$ is the evolution operator with Hamiltonian H. On the other hand, when the cell C associated with F evolves under classical motion, it becomes after time t a new cell C_t to which one can sometimes associate its own approximate projector F_t. Theorem C will express that the operator $\delta F(t) = F(t) - F_t$ is also small under suitable conditions.

Theorem C was conjectured without a proof in I. Analogs of Theorems A and B were stated in III together with a tentative proof using microlocal analysis.[12] I must, however, acknowledge several serious defects of the results published in III: Microlocal analysis is often not familiar to physicists and I did not state precisely the mathematical results I was using. Furthermore, the "proof" used a correspondence between canonical transformations and unitary transformations in cases exceeding what has been rigorously proved.[13] Finally, I only showed that the "small" operators δF were small in the sense of having a small trace, whereas a correct derivation of the logical consequences of Theorems A, B, and C needs a small trace norm, i.e., $\mathrm{Tr}\, |\delta F|$ [with $\delta F = (\delta F\, \delta F^*)^{1/2}$] must be small. Accordingly, a precise statement and a correct proof of these three theorems is still needed and will be given here.

It should be mentioned that Theorem A occurs as a lemma in the derivation of the asymptotic distribution of eigenvalues for a general elliptic operator as investigated by Hörmander.[14] It turns out, however, that Hörmander obtains bounds behaving like $\hbar^{1/3}$ when $\hbar \to 0$, whereas general arguments[7] lead one to expect a behavior in $\hbar^{1/2}$. This is certainly due to the fact that Hörmander was investigating a much more general problem and his lemma was probably the best one that could be obtained to solve this problem, but not the best one for our simpler purpose. This was a reason for trying to get a more direct proof of Theorem A, and it turned out that the proof of Theorem B was a simple consequence of it.

A few words concerning the techniques to be used in the proofs are in order: Microlocal analysis is undoubtedly the mathematical theory best suited to this kind of problems.[2] There is, however, a simple practical substitute for microlocal analysis that is often very useful, namely wavelet expansion.[15] A special case of wavelet expension consists in writing a function as a continuous superposition of Gaussian wave packets and, as such, it has already been much investigated by physicists after the work of Glauber.[6]

So one may choose between a relatively simple and already familiar technique and a more powerful but much more involved general mathematical construction. Expansions in coherent states have been well investigated by physicists, with deep results[6–9] that may be used readily. These were two reasons for choosing to cast the proofs within the language of coherent states. Unfortunately, I was unable to obtain all the needed results by this technique, because apparently wavelet theory is not well suited to an evaluation of trace norms. This is why some recourse to microlocal analysis remained necessary. I have tried to lessen this inconvenience by recalling in the Appendix all the mathematical results that are needed. Perhaps some readers will find them useful for their own problems and will be led to learn more about this deep and beautiful part of mathematics.

The paper is organized as follows. Theorems A and B are stated and proved in Section 2. Theorem C is the subject of Section 3. In Section 4, these results are used to prove rigorously the limit of quantum representations of logic toward classical logic in the conditions where approximate determinism holds. So the present work gives the proof of several key results put forward in I which had remained at the level of more or less intuitive arguments. The Appendix gives the needed essentials of microlocal analysis.

These results will be used in a forthcoming paper to investigate why ergodic systems cannot be reliably described by the Hamilton equations at the classical level, how this difficulty can be alleviated, and what irreversible behavior of such systems occurs as a consequence of the theory.

2. PROJECTORS IN HILBERT SPACE AND CELLS IN PHASE SPACE

Let D and D' be two real, symmetric, $n \times n$ matrices, D being strictly positive definite, their matrix elements having dimension $(\text{length})^{-2} \times$ (action) under a physical change of scale. To the matrix $Q = D + iD'$ we shall associate the following Euclidean metric in phase space:

$$d_Q(x, p) = \frac{1}{4\hbar}(x|\text{Re } Q|x) + \frac{1}{\hbar}(p|\text{Re } Q^{-1}|p) \tag{2.1}$$

and the following family of normalized Gaussian wave packets:

$$g_{(q,p)}(x) = (2\pi)^{-n/4}(\det \text{Re } Q)^{-1/2} \exp[-(1/4\hbar)(x-q|Q|x-q) + ip \cdot x/\hbar] \tag{2.2}$$

It will sometimes be convenient to use two complex matrices A and B in place of Q and Q^{-1}, with the following properties[8]:

(i) A^{-1} and B^{-1} exist.

(ii) BA^{-1} is symmetric.

(iii) The matrix $\text{Re}(BA^{-1})$ is strictly positive definite.

(iv) $(\text{Re } BA^{-1})^{-1} = AA^*$, from which it follows that $(\text{Re } AB)^{-1})^{-1} = BB^*$, together with the family of Gaussian wave packets

$$g'_{(q,p)}(x) = (2\pi)^{-n/4}\hbar^{-n/4}(\det A)^{-1/2} \times \exp[-(1/4\hbar)(x-q|BA^{-1}|x-q) + ip \cdot x/\hbar] \tag{2.3}$$

One can identify the wave packets g_{qp} and g'_{qp} if $Q = 1/2[BA^{-1} + (BA^{-1})^t]$. Conversely, given Q, one can use the form (2.3) with, for instance, $A = (ReQ)^{-1/2}$ and $B = QA$ (nothing is changed if A and B are both multiplied on the right by a unitary matrix with determinant 1).

One will need the scalar product of the two wave packets. It is given by

$$\begin{aligned}\langle g_{q'p'} | g_{pq} \rangle = \exp[&-(1/8\hbar)(q-q' \,|D + D'D^{-1}D'|\, q-q') \\ &+ i(p-p') \cdot (q+q')/2\hbar - (1/2\hbar)(p-p' \,|D^{-1}D'|\, q-q') \\ &- (1/2\hbar)(p-p' \,|D^{-1}|\, p-p')]\end{aligned} \tag{2.4}$$

The Euclidean n-dimensional scalar product is written as $(\cdot)$ and the Hilbert space scalar product as $\langle \cdot \rangle$. Furthermore, one has a decomposition of the identity:

$$I = \int_{R^{2n}} |g_{qp}\rangle\langle g_{qp}| \, dq \, dp \, (2\pi\hbar)^{-n} \tag{2.5}$$

following from the relation $\langle x| \, I \, |y\rangle = \delta(x-y)$, which is easily obtained from an explicit integration.

Let now C be a bounded, connected, and simply connected set C in a phase space $\mathbb{R}^{2n}$ with a boundary ∂C that is piecewise C^2. Given a positive number ε ($\varepsilon < 1$), one will say that *the set C is regular to order ε* if there exists a real, symmetric, $n \times n$ matrix Q and a positive number l such that:

(i) On any C^2 part of ∂C, the curvature radii of ∂C, when computed with the metric d_Q, are all larger than l in absolute value.

(ii) Let $X = (x, p)$ and let $e(x, l)$ be the ellipsoid defined by $g_q(x - \Delta y) \leqslant l^2$. The *margin* of C is defined as the set

$$M = \bigcup_{x \in \partial C} e(x, l) \tag{2.6}$$

It contains ∂C. Let us denote by $[C]$ and $[M]$ the phase space volumes of the sets C and M, where, for instance,

$$[C] = \int_C dx \, dp \tag{2.7}$$

One then assume the condition

$$[M] < \varepsilon[C] \tag{2.8}$$

i.e., a relatively small volume of the margin.

(iii) The numbers l and ε satisfy the relation $e^{-2l^2} < \varepsilon$. (2.9)

Clearly, when $\varepsilon \ll -1$, these conditions imply that one deals with a macroscopic cell, i.e., $[C] \gg (2\pi\hbar)^n$.

As an example, in the case of a cubic cell having a side with length L in the x directions and P in the p directions the best estimates one will find will correspond to $\varepsilon = (\hbar/LP)^{1/2}$ up to a multiplicative constant of order unity.

Let now C be a cell that is regular to order ε and Q a not necessarily real matrix for which C is regular. The operator

$$F = \int_C |g_{qp}\rangle\langle g_{qp}| \, dq \, dp \, (2\pi\hbar)^{-n} \tag{2.10}$$

will be called an *approximate projector* associated with the set C. Its main properties are the following:

1. F is a self-adjoint positive operator, as follows from the property

$$\langle u| F |u\rangle = \int_C |\langle g_{pq} | u\rangle|^2 \, dq \, dp \, (2\pi\hbar)^{-n} \geqslant 0 \tag{2.11}$$

2. Putting $\bar{F} = I - F$ and using the decomposition of the identity (2.5), one gets

$$F = \int_{\bar{C}} |g_{pq}\rangle\langle g_{qp}| \, dx \, dp \, (2\pi\hbar)^{-n} \tag{2.12}$$

$\bar{C}$ is the complementary set of C. The quantity $\bar{F}$ is also a positive operator, so that one has

$$0 \leqslant F \leqslant I \tag{2.13}$$

giving the bound $\|F\| \leqslant 1$.

3. The Hilbert–Schmidt norm of F is given by

$$\|F\|^2_{\mathrm{HS}} = \int_C dq \, dp \, (2\pi\hbar)^{-n} \int_C dq' \, dp' \, (2\pi\hbar)^{-n} \, |\langle g_{qp} | g_{q'p'}\rangle|^2 \tag{2.14}$$

It is finite, as seen from Eq. (2.4), so that F is a compact operator. Its non-zero eigenvalues λ_n are therefore discrete, satisfying

$$0 \leqslant \lambda_n \leqslant 1 \tag{2.15}$$

4. The trace of F is given by

$$\mathrm{Tr}\, F = \int_C dq \, dp \, (2\pi\hbar)^{-n} = [C](2\pi\hbar)^{-n} \tag{2.16}$$

i.e., essentially the number of elementary semiclassical states in the set C.

5. Let us consider the operator

$$\delta F = F^2 - F = \bar{F}F \tag{2.17}$$

One can easily estimate its trace norm, i.e., the quantity $\mathrm{Tr}\, |\delta F|$, where $|\delta F|$ is the absolute value operator $(\delta F \, \delta F)^{1/2}$. In fact, from

$$\delta F = \int_{\bar{C}} dq \, dp \, (2\pi\hbar)^{-n} \int_C dq' \, dp' \, (2\pi\hbar)^{-n} \, |g'\rangle\langle g| (\langle g' | g\rangle) \tag{2.18}$$

one gets

$$\mathrm{Tr}\,|\delta F| \leqslant \int_{\bar{C}} \int_{C} dq'\, dp'\, (2\pi\hbar)^{-n}\, dq\, dp\, (2\pi\hbar)^{-n} |\langle g' \mid g \rangle|^2 \qquad (2.19)$$

Under the regularity assumptions, one can estimate this double integral by integrating one variable over R^{2n} and the other one over the margin of C, so that

$$\mathrm{Tr}\,|\delta F| < c[M](2\pi\hbar)^{-n} \qquad (2.20)$$

or

$$(\mathrm{Tr}\,|\delta F|/\mathrm{Tr}\,F) < c\varepsilon \qquad (2.21)$$

c is a constant of order unity.

Given a regular set C, one can in general associate with it many approximate projectors corresponding to a different choice for the matrix Q and the associated metric. One needs to prove the equivalence of two such approximate projectors F_1 and F_2, meaning that the corresponding trace norm $\mathrm{Tr}\,|F_1 - F_2|$ is of order ε. This property is harder to prove than the previous ones and the proof to be given will use microlocal analysis.

Using Eq. (A.2) of the Appendix, one obtains the Weyl symbol $f(x, \xi)$ of the operator F:

$$\begin{aligned} f(x, \xi) = \int_C dq\, dp\, (2\pi\hbar)^{-n} \exp\{&-(x-q\ |D|\ x-q)/2\hbar \\ &-[p-\xi-DD'(x-q)\ |D^{-1}|\ p-\xi-DD'(x-q)]/2\hbar\} \end{aligned} \qquad (2.22)$$

It is seen that $f(x, \xi)$ is practically equal to 1 or zero outside M, up to exponentially small corrections smaller than e^{-l2}. The function $f(x, \xi)$ satisfies the conditions for being a symbol of arbitrarily negative order.

Given two such symbols f_1 and f_2 corresponding to the same set C and two different matrices $Q_1 = D_1 + iD'_1$ and $Q_2 = D_2 + iD'_2$, the trace norm of the operator $F_1 - F_2$ can be estimated from the symbols, using Theorem A.4. The function $f_1 - f_2$ is significantly different from zero only in the union $M_1 \cup M_2$ of the two corresponding margins. Neglecting corrections of higher order in $\hbar$, one finds for $\mathrm{Tr}\,|F_1 - F_2|$ the estimate

$$\int_{R^{2n}} dx\, d\xi\, (2\pi\hbar)^{-n}\, |f_1(x, \xi) - f_2(x, \xi)| \qquad (2.23)$$

of order $([M_1] + [M_2])(2\pi\hbar)^{-n}$. Assuming that both matrices Q_1 and Q_2 allow the set C to be regular to order ε, one gets

$$\mathrm{Tr}\,|F_1 - F_2|/\mathrm{Tr}\,F_1 < c\varepsilon \qquad (2.24)$$

c is a constant of order unity. To summarize, one has obtained the following result.

Theorem A. Let C be a set in phase space that is regular to order ε for some matrix Q. One can then define an associated approximate projector, namely an operator F that is self-adjoint, compact with all its eigenvalues in $[0, 1]$, having a trace as given by Eq. (2.16) and such that the operator $\delta F = F^2 - F$ has a trace norm of order $\varepsilon \cdot \operatorname{Tr} F$.

Furthermore, the difference $F_1 - F_2$ of two such approximate projectors also has a trace norm of order $\varepsilon \cdot \operatorname{Tr} F$.

It is interesting to find the smallest value of ε (as far as orders of magnitude are concerned) that one can assign to a given set C in phase space. For definiteness, let it be assumed that one can introduce a reference length L and a reference momentum P such that $LP \gg 2\pi\hbar$, the curvature radii of ∂C being all of order unity in the metric

$$g_0(dx, dp) = L^{-2}\, dx^2 + P^{-2}\, dp^2 \tag{2.25}$$

and, furthermore, when C has the shape of a box, the distance of a face to a nonadjacent one being also of order unity. This is a very special case, but any other specific example can be treated along the same lines. It will also be assumed that ∂C is C^∞ except on the edges if they exist. This assumption is not necessary, although rather convenient.

One will use microlocal analysis and only the case of no edge will be treated, the case of a box-shaped region being technically slightly more involved.

Let $f(x, \xi)$ be a smoothed characteristic function for the set C. This is a C^∞ function identically equal to 1 or 0 except in a transition region containing ∂C of small width Δ (in the dimensionless metric g_0) to be called again the margin M of C. In M, $f(x, \xi)$ passes continuously from the value 1 well inside C to the value 0 well outside C. Its seminorms $C_{\alpha\beta}$ are of order $\Delta^{-(|\alpha| + |\beta|)/2}$ except for numerical constants.

Lemma 1. The operator F having the Weyl symbol $f(x, \xi)$ satisfies the following properties:

a. It is a self-adjoint compact operator.

b. Its eigenvalues satisfy the inequalities

$$-\varepsilon_1 < f_n < 1 + \varepsilon_2$$

where ε_1 and ε_2 are of order $\Delta^{-4}(\hbar/LP)^2$.

Sketch of the Proof. Property a follows from Theorem A.1 and property b from Theorem A.3.

Lemma 2. Let $\delta F = F^2 - F$. The trace norm of this operator is bounded by the supremum of $K[M](2\pi\hbar)^{-n}$ and $K'[M](2\pi\hbar)^{-n}\Delta^{-4}(\hbar/LP)^2$ as long as $\Delta \gg (\hbar/LP)^{1/2}$, K and K' being numerical constants of order unity.

Sketch of the Proof. The function $\delta_1 f = f^2 - f$ is zero outside M. Inside f, one has $|\delta_1 f| < 1/4$, so that, using Theorem A.4, the trace norm of the associated operator $\delta_1 F$ satisfies

$$\mathrm{Tr}\,|\delta_1 F| < K[M](2\pi\hbar)^{-n}$$

up to correction of higher order in $\hbar$.

Let $d(x, \xi)$ be the symbol of the operator $F^2 - F$. According to Theorem A.2, one has

$$d(x, \xi) = f^2(x, \xi) - (\hbar^2/8)\, f\{\cdot\}^2 f = \delta_1 f + \delta_2 f$$

leaving out corrective terms of higher order in $\hbar$. This is permissible as long as $\Delta \gg (\hbar/LP)^{1/2}$. Now $\delta_2 f$ vanishes also outside M and is of order $(\hbar/LP)^{21}\Delta^{-4}$ times a finite constant, so that, using once again Theorem A.4, one gets

$$\mathrm{Tr}\,|\delta_2 F| < K'[M]\Delta^{-4}(\hbar/LP)^2(2\pi\hbar)^{-n}$$

These results show that, using this alternative definition of a projector, one can go down to a value of ε in the inequality

$$\mathrm{Tr}\,|F^2 - F| < K[M](2\pi\hbar)^{-n} = \varepsilon$$

of the order of $\varepsilon = (\hbar/LP)^\alpha$ with $\alpha > 1/2$.

With trivial changes and using smoothed characteristic functions to define a projector, one can also obtain the following result.

Theorem B. Let C_1, C_2, and $C_1 \cap C_2$ be three sets in phase space, all having C^∞ boundaries with curvature radii of order unity in the metric g_0 except on a finite number of edges, and let F_1, F_2, and F_{12} be approximate projectors for each of them that are obtained from a smoothed characteristic function. Then the operator

$$\delta F = F_1 F_2 - F_{12}$$

is bounded in trace norm by

$$\mathrm{Tr}\,|\delta F| < K[C](2\pi\hbar)^{-n}(\hbar/LP)^\alpha \tag{2.26}$$

where $[C] = \sup([C_1], [C_2])$, $\alpha > 1/2$, and K a constant of order unity.

This theorem immediately gives a bound for the commutator $[F_1, F_2]$.

3. DYNAMICAL EVOLUTION OF PROJECTORS

In the present section, we shall use approximate projectors coming from a superposition of coherent state projectors. The results are also probably true for projectors generated by smoothed characteristic functions, but no complete proof is available. Such a proof would amount to an extension of Egorov's theorem[13] to a larger class of canonical transformations, although with a much more restricted class of operators. A proof using microlocal analysis would also presumably allow one to consider the case of rather general Hamilton functions and configuration space not reduced to $\mathbb{R}^n$. However, the method to be used here will be restricted to Hamiltonian operators of the form

$$H = \sum_{j=1}^{n} p^2/2m + V(x_1,..., x_n) \tag{3.1}$$

It would of course be easy to introduce different mass coefficients for the different degrees of freedom, but the form (3.1) is enough to illustrate the main physical aspects of the problem.

The potential V is assumed to satisfy the following conditions:

(i) $V \in C^2(\mathbb{R}^n)$, $|V(x)| \leqslant K_1 e^{Mx2}$, $V(x) \geqslant -K_2$ $(K_1 > 0,\ K_2 \geqslant 0,\ M \geqslant 0)$.

(ii) Let $V^{(2)}(x) = (\partial/\partial x_j\, \partial/\partial x_k)\, V(x)$ be the Hessian matrix of V and $\| V^{(2)}(x)\|$ its operator norm as a matrix (i.e., the absolute value of its largest eigenvalue). $V^{(2)}(x)$ is uniformly Lipschitz on compact subsets of $\mathbb{R}^n$, i.e., given any $A > 0$, there exists β such that $\| V^{(2)}(x) - V^{(2)}(y)\| \leqslant \beta |x-y|$ for $|x| < A$ and $|y| < A$.

Coherent states will be expressed in the form (2.9). Such a wave packet depends upon several parameters: an average position q, an average momentum p, and two dispersion matrices A and B satisfying the conditions given in Section 2.

Let $g_{qp(0)}$ be such a wave packet. It is convenient to introduce classically transported wave packets $g_{qp(t)}$, still Gaussian, with their parameters (q, p, A, B) depending upon time and satisfying the following differential equations:

$$dp_j/dt = -(\partial V/\partial x_j)(q(t)) \tag{3.2a}$$

$$dq_j/dt = p_j(t)/m \tag{3.2b}$$

$$dA/dt = iB(t)/m \tag{3.3a}$$

$$dB/dt = 2iV^{(2)}(q(t))\, A(t) \tag{3.3b}$$

Equations (3.2a) and (3.2b) are the classical equations of motion for a trajectory $(q(t), p(t))$. In Eq. (3.3b), the right-hand side is a matrix product. Equations (3.3a) and (3.3b) define a classical transport for the uncertainties in position and momentum, starting from initial matrices A_0, B_0 at time zero. In fact, the correlation matrices for position and momentum are given, respectively, by

$$\langle (x_j - \langle x_j \rangle)(x_k - \langle x_k \rangle) \rangle = (\hbar/2)(AA^* + A^*A)_{jk} \tag{3.4a}$$

$$\langle (p_j - \langle p_j \rangle)(p_k - \langle p_k \rangle) \rangle = (\hbar/8)(BB^* + B^*B)_{jk} \tag{3.4b}$$

Given an initial point (q_0, p_0) in phase space at time zero, the corresponding classical action $S(t)$ is defined by

$$S(t) = \int_0^t [p(t')^2/2m - V(q(t'))] \, dt' \tag{3.5}$$

In the expression (2.3) of the wave packet $g_{qp(t)}$ there enters a normalization factor $[\det A(t)]^{-1/2}$, where the square root never vanishes and is defined by continuity (this takes care of the Maslov index[16]). With these conditions and conventions, one has the following result.

Theorem (Hagedorn[8]). For each time $T > 0$ and each positive $\lambda < 1/2$, there exist positive constants K and δ such that, whenever $|t| < T$ and $\hbar < \delta$, one has

$$\| e^{-iHt/\hbar} g_{qp(0)} - e^{iS(t)/\hbar} g_{qp(t)} \| \leqslant K\hbar^{\lambda} \tag{3.6}$$

In fact, one has exactly $K = 0$ when V is a polynomial of degree 2 (constant force + harmonic oscillator). A rough estimate of the right-hand side in inequality (3.6) is given by

$$\hbar^{1/2} \int_0^t |V^{(3)}(t)| \, a^3(t) \, dt \tag{3.7}$$

where $V^{(3)}(t)$ represents the largest component of the tensor $\partial_i \partial_j \partial_k V(x)$ at the classical position $q(t)$ and $a^2(t)$ is the largest eigenvalue of the matrix $D^{-1}(t)$ related to $A(t)$ as explained in Section 2.

Let C_0 be an initial set in phase space at time zero, regular for the matrix Q_0 to order ε. Let C_t be the image of C_0 under classical motion at time t. It will be assumed that C_t is also regular to order ε for all the matrices $Q(t)$ related to Q_0 for any point (q_0, p_0) belonging to the interior of C_t as long as $0 < t < T$ $(T > 0)$. Furthermore, assume that $K\hbar^{\lambda} < \varepsilon$ uniformly in C_0 in Eq. (3.6). Given C_0 and Q_0, the regularity of C_t can in principle be checked by a calculation using classical dynamics and I shall not try to give an analytic criterion. The bound upon $K\hbar^{\lambda}$ is more difficult to assert, but if the estimate (3.7) is used, it again boils down to a condition involving only classical dynamics. When these conditions are satisfied, it will be said that *dynamics is regular to order* ε for the cell C_0 during the time interval $(0, T)$.

Then Hagedorn's theorem yields a simple corollary that is most useful for the interpretation of quantum mechanics:

Theorem C. Let C_0 be a cell regular to order ε and let dynamics be regular to order ε for C_0 during the time interval $(0, T)$. Let F_0 (resp. F_t) be an approximate projector associated with the cell C_0 (resp. C_t) using Eq. (2.10). Let $F(t) = U(t)\, F_0\, U^{-1}(t)$ and

$$\delta F(t) = F(t) - F_t \tag{3.8}$$

Then one has

$$\mathrm{Tr}\, |\delta F(t)| < K\varepsilon(\mathrm{Tr}\, F_0) \tag{3.9}$$

K is a constant of order unity.

Proof. Let F_t' be the projector associated with C_t by Eq. (2.10) using the wave packets $g_{qp(t)}$. Despite the dependence of the matrices $A(t)$, $B(t)$ over the initial point (q_0, p_0), Eq. (2.10) still defines a projector. This is most easily seen as follows: Define an operator F_t' by Eq. (2.10), where the dispersion matrices (A, B) depend upon (p, q). One can compute the Weyl symbol $f_t'(x, \xi)$ of this operator, using Eq. (A.2). The integration over the variable y in Eq. (A.2) can be evaluated explicitly to show that $f_t'(x, p)$ is equal to 1 within C_t, and to zero outside, except in a small transition region that is a margin. Then, using Theorem A.3, this evaluation can be used to show that F_t' is an approximate projector.

If the projector F_t uses other wave packets with a fixed dispersion, inequality (2.24) gives

$$\mathrm{Tr}\, |F_t' - F_t| < c\varepsilon\, \mathrm{Tr}\, F_t \tag{3.10}$$

Furthermore, Eq. (2.16) together with the equality $[C_0] = [C_t]$ resulting from Liouville's theorem gives $\mathrm{Tr}\, F_t = \mathrm{Tr}\, F_0$. Therefore, one can consider only the operator $\delta' F(t) = F(t) - F_t'$.

Writing

$$e^{-iSt/(\hbar)}\delta g_{qp,t} = e^{-iHt/\hbar} g_{pq(0)} - e^{-iS(t)/\hbar} g_{pq(t)} \tag{3.11}$$

one gets

$$\begin{aligned} F(t) - F_t' = &\int_{C_0} dq_0\, dp_0\, (2\pi\hbar)^{-n}\, |g_{pq(t)} + \delta g_{pqit}\rangle\langle g_{pq(t)} + \delta g_{pq,t}| \\ &- \int_{C_t} dq\, dp(t)(2\pi\hbar)^{-n}\, |g_{pq(t)}\rangle\langle g_{pq(t)}| \end{aligned} \tag{3.12}$$

A change of variables $(q_0, p_0) \to (q(t), p(t))$ with Jacobian unity then gives, after suppressing the unnecessary time index,

$$F(t) - F_t' = \int_{C_t} dq\, dp\, (2\pi\hbar)^{-n}(|g_{pq} + \delta g_{pq}\rangle\langle g_{pq} + \delta g_{pq}| + |g_{pq}\rangle\langle g_{pq}|) \tag{3.13}$$

The term $[F(t) - F_t']^{(1)}$ linear in δg_{pq} is bounded in trace norm by

$$\begin{aligned}
[F(t) - F_t']^{(1)}_{\mathrm{Tr}} &\leqslant \int_{C_t} 2\, dq\, dp\, (2\pi\hbar)^{-n} | \langle g_{pq}\| \cdot \|\delta g_{pq}\rangle) \\
&\leqslant \int_{C_t} 2\, dq\, dp (2\pi\hbar)^{-n}\, \|g_{pq}\| \cdot \|\delta g_{pq}\| \\
&\leqslant 2\varepsilon[C_t](2\pi\hbar)^{-n} = 2\varepsilon \operatorname{Tr} F_t = 2\varepsilon \operatorname{Tr} F_0
\end{aligned} \tag{3.14}$$

The term quadratic in δq_{pq} is bounded by

$$\begin{aligned}
\|F(t) - F_t'\|^{(2)}_{\mathrm{Tr}} &\leqslant \int dq\, dp\, (2\pi\hbar)^{-n}\, \|\delta g_{pq}\|^2 \\
&\leqslant \varepsilon^2 \operatorname{Tr} F_0
\end{aligned} \tag{3.15}$$

Inequalities (3.10), (3.14), and (3.15) give (3.9).

Theorem C may be considered as stating sufficient conditions for identifying quantum dynamics and logic to classical dynamics and logic up to a relative error in probability of order ε. The smallest value of ε one may get in a given situation is controlled by data computable by classical dynamics, except for the right-hand side of inequality (3.6), which may, however, be estimated by the quantity (3.7).

Although Theorem C only gives sufficient conditions, it may be expected that the connection with classical physics will be lost when the uncertainties become uniformly large and/or when the boundary ∂C_t becomes so irregular that there is no possible way to associate an approximate projector with C_t. It may be shown that the canonical transformation $(q_0, p_0) \to (q(t), p(t))$ has finite first derivatives, i.e., the differentials $\partial q(t)/\partial q_0$, $\partial q(t)/\partial p_0$, $\partial p(t)/\partial q_0$, and $\partial p(t)/\partial p_0$ exist. Accordingly, the time evolution for the uncertainties (3.3) can be solved[8] to give

$$\begin{aligned}
A(t) &= [\partial Q(t)/\partial q_0] A_0 + (i/2)[\partial q(t)/\partial p_0] B_0 \\
B(t) &= -2i[\partial p(t)/\partial q_0] A_0 + [\partial p(t)/\partial p_0] B_0
\end{aligned} \tag{3.16}$$

There is one case where it can be expected that the connection with classical physics is completely lost, namely when the derivatives of

$(q_0, p_0) \to (q(t), p(t))$ increase exponentially with time, since both the uncertainties and the boundary become uncontrollable after a finite time. This is a very interesting point, since it shows that the reliability of classical physics, except during a finite time, is quite questionable when one is dealing with some ergodic or Lyapunov unstable systems. It means that for such a system, the classical Hamilton equations lead to classical histories which have no meaning in any underlying quantum logic. In other words, the link between quantum mechanics and classical mechanics is not universal. This question will be further investigated in a forthcoming paper.

On the other hand, if one considers a regular macroscopic system, using only a few collective coordinates to describe it as happens for the apparatus that engineers and physicists build or other reasonably stable macroscopic systems, one may expect that quantum dynamics and quantum logic are well approximated by classical dynamics and classical logic with errors in probability of the order of $\hbar^{1/2}$ or so.

These are the systems for which the theory proposed in I are valid and they include what one usually means by a measuring apparatus or a reliable record (as, for instance, the fossil track of an α-particle in a rock).

4. CONSEQUENCES

The present results control in practice the approximation of quantum logic by classical logic.

Consider the following example. A physical system S has only continuous degrees of freedom or one is considering a model for S involving only some continuous collective coordinates. Let C_0, C_1, and C_2 be three cells in phase space satisfying the following asumptions: The dynamics is supposed to be regular for C_0 and C_1 up to order ε during time interval T. Classical motion transforms the initial cell C_0 at time zero into a cell $C_0(t_1)$ at time t_1 and assume $C_1 \subset C_0(t_1)$. Similarly, classical motion transforms C_1 at time t_1 into the cell C_2 at time t_2 $(0 < t_1 < t_2 < T)$. Assuming in the logic of classical dynamics that the system is initially in a state described by the cell C_0, one would say that it can be in C_1 at time t_1 and, *if* so, *then* it must be in C_2 at time t_2, i.e., $[C_2, t_2] \Rightarrow [C_1, t_1]$, these propositions belonging to classical logic and the implication following from the interpretation of classical logic by set theory in the universe of discourse of classical dynamics.

Assuming, however, that classical dynamics and classical logic are of no fundamental avail, but should rather be considered as approximations to quantum dynamics and quantum logic, one is led to reconsider the above statements in a new light: Let F_0, F_1, F_2 be, respectively, approximate projectors of order ε associated with the cells C_0, C_1, C_2. Let the initial state operator be given by $\rho = F_0/(\mathrm{Tr}\, F_0)$. Let $[C_1, t_1]$ denote the *quantum* proposition asserting that the system is in the cell C_1 at time t_1. To be precise, it should be recalled that a quantum logical predicate has in general the form $[S, A, B]$, asserting that some observable A describing the system S is in some part B of the spectrum σ_A. Here the quantum predicate $[C_1]$ is interpreted as $[F_1, [1-\varepsilon, 1]]$, meaning that the observable F_1 has its value in the part of its spectrum belonging to the interval $[1-\varepsilon, 1]$. Clearly, this kind of classically meaningful predicate involves some fuzziness, since there is some arbitrariness in the choice of the approximate projector F_1 and of the interval $[1-\varepsilon, 1]$, but this is precisely the kind of imprecision one may expect in the relation between classical physics and quantum physics. It should be noticed that the strict projector E_1 associated with the predicate $[F_1, [1-\varepsilon, 1]]$ differs from F_1 itself by an operator having a trace norm smaller than ε. Therefore, for calculations to be made with error ε, one can as well use F_1 for the projector associated with the predicate $[C_1]$. Furthermore, with the time-indexed predicate $[C_1, t_1]$, one will associate the projector $F_1'(t_1) = U^{-1}(t_1)\, F_1\, U(t_1)$. Similar conventions will be used for $[C_2, t_2]$. The projector representing the negation $[C_1^*]$, C_1^* being the set complementary to C_1 in phase space, is similarly associated with the projector $F_1^* = I - F_1$.

There is only one logical consistency condition[17] for the smallest Griffiths family of history predicates containing both predicates $[C_1, t_1]$ and $[C_2, t_2]$, that is,

$$\mathrm{Tr}\{[F_1(t_1), [\rho, F_1^*(t_1)]\, F_2(t_2)\} = 0 \tag{4.1}$$

It is useful to define a reference scale for the probabilities or the traces, which will be conveniently defined as

$$\begin{aligned} w_0 &= \mathrm{Tr}[F_1(t_1)\, \rho F_1(t_1)\, F_2(t_2)] \\ &= \mathrm{Tr}[F_1\, U(t_1)\, F_0 U^{-1}(t_1)\, F_1 U^{-1}(t_2 - t_1)\, F_2 U(t_2 - t_1)]/\mathrm{Tr}\, F_0 \end{aligned} \tag{4.2}$$

According to Theorem C, $U(t_1)\, F_0 U^{-1}(t_1)$ is, up to errors of order ε in the norm, an approximate projector associated with $C_0(t_1)$. Its product by F_1 both on the right and the left is, with the same error, simply an approximate projector associated with C_1 according to Theorem B. One can neglect these terms having a trace norm of order ε in Eq. (4.2) because all the factors are projectors having an operator norm unity, so that the inequality

$$|\mathrm{Tr}(AB)| \leqslant \mathrm{Tr}\, |A| \cdot \|B\|$$

shows that one is only making an error ε in w_0. This being seen, one finds that with an error of order ε, one has

$$w_0 = \mathrm{Tr}[U(t_2 - t_1)F_1 U^{-1}(t_2 - t_1)F_2]/\mathrm{Tr}\, F_0$$

Using Theorem C, one gets immediately

$$w_0 = (\mathrm{Tr}\, F_1)/(\mathrm{Tr}\, F_0) + O(\varepsilon) \tag{4.3}$$

The trace occurring in the consistency condition (4.1) can be evaluated along the same lines to give

$$\mathrm{Tr}\{[F_1(t_1)[\rho, F_1^*(t_1)]]\, F_2(t_2)\} = O(\varepsilon) \tag{4.4}$$

It may be useful to insert here a remark without giving a proof, which would need quite different considerations: the right-hand side of Eq. (4.4) is extremely sensitive to the exact choice one makes for the boundaries of the cells or the approximate projectors. In practice, it may take positive or negative values with an absolute value of order ε (examples are given in II). Any kind of averaging then replaces the term $O(\varepsilon)$ in Eq. (4.4) by $O(\varepsilon^2)$. In any case the consistency conditions are satisfied at least to order ε (in practice to order ε^2) and one can use the rules of Boolean logic with errors in probability of order ε.

The probability of the predicate $[C_2, t_2]$ is given by

$$w' = \mathrm{Tr}[\rho F_2(t_2)]/\mathrm{Tr}\, F_0 \tag{4.5}$$

and an analysis similar to the preceding one gives

$$w' = (\mathrm{Tr}\, F_2)/(\mathrm{Tr}\, F_0) + O(\varepsilon) = (\mathrm{Tr}\, F_1)/(\mathrm{Tr}\, F_0) + O(\varepsilon) = w_0 + O(\varepsilon) \tag{4.6}$$

Similarly, one gets

$$w'' = \mathrm{Tr}[\rho F_1(t_1)]/(\mathrm{Tr}\, F_0) = w_0 + O(\varepsilon) \tag{4.7}$$

The near equality these three probabilities w_0, w_1', and w'' together with the consistency conditions immediately yields the following two *quantum* logical implications that are valid up to errors of order ε:

$$[C_1, t_1] \Rightarrow [C_2, t_2] \tag{4.8a}$$

$$[C_2, t_2] \Rightarrow [C_1, t_1] \tag{4.8b}$$

Therefore one has found complete agreement (up to order ε) between the predictions of classical logic and those of quantum logic, as announced in less precise terms in I. The general pattern of such proofs should be clear enough to show that such an agreement always occurs when the conditions of applicability for Theorems A and C are satisfied, i.e., when the cells are regular enough and the dynamics is regular.

APPENDIX. PSEUDO-DIFFERENTIAL OPERATORS

There is not yet an account of microlocal analysis directed toward physicists. This is why I give here a summary of the results used in the present paper. They have been translated from more general theorems to be found in Hörmander's book.[12] Their proofs are most often extremely involved and they will not be given here except for a few hints to show how the results arise. I hope that this brief account will be found useful by some physicists for other problems.

A.1. Operators and Associated Functions

Let a physical system be described by the coordinates $x=(x_1,\dots,x_n)$ in the configuration space $\mathbb{R}^n$. The momentum coordinates will be denoted for convenience by the corresponding Greek letter $\xi=(\xi_1,\dots,\xi_n)$. The Hilbert space of quantum mechanics for this system is $\mathscr{H}=L^2(\mathbb{R}^n)$.

Let Ω be some operator in $\mathscr{H}$; its kernel $\Omega(x, y)$ is by definition the function or distribution

$$\Omega(x, y)=\langle x\,|\Omega|\,y\rangle \tag{A.1}$$

which may or may not exist.

A function $\omega(x, \xi)$ defined on the phase space $\mathbb{R}^{2n}$ will be associated with the operator Ω; it is defined by the partial Fourier transform

$$\omega(x, \xi)=\int \Omega(x+y/2, x-y/2)\exp(-i\xi\cdot y/\hbar)\,dy \tag{A.2}$$

where $\xi\cdot x=\xi_1\cdot x_1+\cdots+\xi_n\cdot x_n$. The conditions on the function $\omega(x, \xi)$ and the operator Ω allowing such a correspondence will be given latter. The same letter, either capital or in lower case, will be used systematically to denote an operator and the associated function.

Equation (A.2) shows that the adjoint operator Ω^+ corresponds to the complex conjugate function $\omega^*(x, \xi)$, so that a real function corresponds to a self-adjoint operator. Let X_j and P_j denote the position and momentum component operators; the corresponding functions are, respectively, x_j and ξ_j. To the identity operator corresponds the function 1 identically equal to unity, and the function identical to zero corresponds to the zero operator. To a particle Hamiltonian operator

$$H = \sum_j (P_j^2/2m_j) + V(X) \tag{A.3}$$

corresponds the Hamilton function

$$h(x, \xi) = \sum_j (\xi_j^2/2m_j) + V(x) \tag{A.4}$$

The action of an operator Ω on a wave function $u(x)$ is given as a result of Eqs. (A.1) and (A.2) by

$$(\Omega u)(x) = \int \omega((x+y)/2, \xi) \exp[i\xi \cdot (x-y)/\hbar]\, u(y)\, dy\, d\xi/(2\pi\hbar)^n \tag{A.5}$$

When the trace of Ω exists, the same equations give

$$\operatorname{Tr} \Omega = \int \omega(x, \xi)\, dx\, d\xi/(2\pi\hbar)^n \tag{A.6}$$

These conventions constitute the basis of the Weyl calculus[18] that is a version of the theory of pseudo-differential operators.[12] They are well known in statistical physics under another guise, where Ω stands for a density operator and $\omega(x, \xi)$ for the associated Wigner distribution function.[19]

A.2. Symbols

One is interested in semiclassical physics, i.e., in wave functions or operators varying slowly on the quantum scale $\hbar$. Rather than wave functions, it will be convenient to deal with density operators or projectors. The slow variation of a density operator ρ is most easily defined as a property of its associated function $\rho(x, \xi)$: if L is a typical length and P a typical momentum for the variation of $\rho(x, \xi)$, then one assumes that

$$LP \gg \hbar$$

It will be convenient to fix these scales (L, P) once and for all for a given problem and the following two functions will be used to characterize a slow variation:

$$\begin{aligned} \mu(x, \xi) &= (1 + x^2/L^2 + \xi^2/P^2)^{1/2} \\ k(x, \xi) &= (\hbar/LP)(1 + x^2/L^2 + \xi^2/P^2)^{-1} \end{aligned} \tag{A.7}$$

Given any real number m, a function $\omega(x, \xi)$ will be called a symbol of order m if it is indefinitely differential (aC^∞ function) and is bounded as well as its derivatives in the following form:

$$|\partial_x^\alpha \partial_\xi^\beta \omega(x, \xi)| \leqslant C_{\alpha\beta} L^{-|\alpha|} P^{-|\beta|} \mu(x, \xi)^{m-|\alpha|-|\beta|} \tag{A.8}$$

The notation is the following: α, for instance, is a multi-index $\alpha = (\alpha_1, ..., \alpha_n)$, $\alpha_j \geqslant 0$ whatever j. The notation ∂_x^α represents the differential operator $(\partial/\partial x_1)^{\alpha_1} \cdots (\partial/\partial x_n)^{\alpha_n}$. The quantities $C_{\alpha\beta}$ are constants, which are called the seminorms of $\omega(x, \xi)$, and their values give a precise meaning to what is meant by the slow variation of $\omega(x, \xi)$. Most often the constants L and P will be chosen so that the seminorms will be of the order of unity. The class of all symbols of order m is denoted by S^m. The operators that can be associated with symbols are called pseudo-differential operators.

For instance, the components of the position operator X and the momentum operator P are pseudo-differential operators. Their symbols belong to S^1. The kinetic energy in Eq. (A.4) belongs to S^2. The Hamilton function is a symbol only if the potential is itself a symbol. This is a rather strong assumption, since it implies in particular that it is a C^∞ function. It excludes the case of the Coulomb potential, which is not-everywhere differentiable. However, this important special case can be handled by more refined techniques.[20]

One sometimes needs another kind of symbol: Semiclassical physics is generally expressed by expansions in powers of $\hbar$ and in the present case by expansions in powers of the dimensionless parameter $(\hbar/LP)$. It will be convenient to use a shorthand notation for the functions or operators occurring in such a series. A C^∞ function $\omega(x, \xi)$ will be said to belong to the class of symbols $S^m(k^N)$ if it satisfies the bounds

$$|\omega(x, \xi)| \leqslant C'_{\alpha\beta} L^{-|\alpha|} P^{-|\beta|} k^N(x, \xi)\, \mu(x, \xi)^{m-|\alpha|-|\beta|} \tag{A.9}$$

When the constants $C'_{\alpha\beta}$ are of order unity, the small factor $(\hbar/LP)$ occurring in the function $k(x, \xi)$ tells us how small the function $\omega(x, \xi)$ is. Knowing in such a case that a function belongs to the class $S^m(k^N)$ therefore tells us that it is at most of order $(\hbar/LP)^N$, that it varies typically over distances of order (L, P), and how it behaves when $|x|$ and $|\xi|$ tend to infinity.

The fact that a symbol $\omega(x, \xi)$ belongs to a given class S^m often gives very useful information concerning the properties of the associated operator:

Theorem A.1. Let $\omega(x, \xi)$ belong to S^m. Then, if $m \leqslant 0$, the associated operator Ω is bounded. If $m < 0$, Ω is compact.

As is well known, a compact operator has only discrete and bounded nonzero eigenvalues.

A.3. Products of Operators

Some properties of the correspondence between symbols and operators are obvious: sums as well as products by pure numbers do correspond. The product of two operators is much more difficult to handle. Consider two operators A_1 and A_2 with respective symbols $a_1(x, \xi)$ and $a_2(x, \xi)$ belonging to the classes S^{m_1} and S^{m_2}. The problem is to find what symbol $b(x, \xi)$ corresponds to the operator product product $B = A_1 A_2$.

It will be convenient to introduce the Fourier transform of a wave function $u(x)$ through

$$\begin{aligned} \hat{u}(\xi) &= \int \exp(-i\xi \cdot x/\hbar)\, u(x)\, dx \\ u(x) &= \int \exp(i\xi \cdot x/\hbar)\, \hat{u}(\xi)\, d\xi/(2\pi\hbar)^n \end{aligned} \tag{A.10}$$

as well as the complete Fourier transform of a symbol with respect to both arguments

$$\begin{aligned} \hat{a}(\eta, y) &= \int a(x, \xi) \exp[i(\xi \cdot y - \eta \cdot x)/\hbar]\, dx\, d\xi (2\pi\hbar)^{-n} \\ a(x, \xi) &= \int \hat{a}(\eta, y) \exp[-i(\xi \cdot y - \eta \cdot x)/\hbar]\, dy\, d\eta\, (2\pi\hbar)^{-n} \end{aligned} \tag{A.11}$$

A straightforward computation using Eq. (A.5) gives

$$\begin{aligned} b(x, \xi) = \int & a_1(x + z, \xi + \zeta)\, a_2(x + t, \xi + \tau) \\ & \times \exp[2i\sigma(t, \tau; z, \zeta)/\hbar]\, dz\, d\zeta\, dt\, d\tau/(\pi\hbar)^{2n} \end{aligned} \tag{A.12}$$

where σ denotes the antisymmetric bilinear form (symplectic form)

$$\sigma(t, \tau; z, \zeta) = \tau \cdot z - \zeta \cdot t \tag{A.13}$$

Equation (A.12) can be written in terms of the Fourier transforms of the symbols a_1 and a_2 as

$$\begin{aligned} b(x, \xi) = \int & e^{i(\eta \cdot x - \xi \cdot y)/\hbar}\, dy\, d\eta\, (2\pi\hbar)^{-n} \int \hat{a}_1(\zeta, z)\, \hat{a}_2(\tau, t)\, \delta(\xi + \tau - \eta) \\ & \times \delta(z + t - y) e^{i(\zeta \cdot t - \tau \cdot z)/2\hbar}\, dz\, d\zeta\, dt\, d\tau\, (2\pi\hbar)^{-n} \end{aligned} \tag{A.14}$$

Expanding the last exponential as a series and identifying, for instance, a multiplication of $\hat{a}_1(\zeta, z)$ by ζ or z as a derivation acting upon $a_1(x, \xi)$, it is possible to write Eq. (A.14) in a much more transparent form. A few notational conventions are necessary to do so.

The Poisson bracket of two functions f and g is defined by

$$\{f, g\} = \partial_\xi f \cdot \partial_x g - \partial_x f \cdot a_\xi g$$

One can more generally define a Poisson bracket differential operator $\{\cdot\}$ by

$$\{\cdot\} = \langle - \partial_\xi \cdot \partial_x \rightarrow - \langle - \partial_x \cdot \partial_\xi \rightarrow$$

the direction of the arrow indicating wether the corresponding differentiation acts upon a function on the right or on the left. For instance, one has

$$f\{\cdot\}g = \{f, g\}$$

$$f\{\cdot\}^2 g = \sum_{jk} [(\partial^2 f/\partial\xi_j\,\partial\xi_k)(\partial^2 g/\partial x_j\,\partial x_k) + (\partial^2 f/\partial x_j\,\partial x_k)(\partial^2 g/\partial\xi_j\,\partial\xi_k) - 2(\partial^2 f/\partial x_j\,\partial\xi_k)(\partial^2 g/\partial\xi_j\,\partial x_k)]$$

and so on. An exponential of the Poisson bracket operator can then be defined as

$$\exp(\lambda\{\cdot\}) = \sum_{r=0}^{\infty} (1/r!)\,\lambda^r\{\cdot\}^r$$

Using this notation, one can then write the symbol of an operator product as given by Eq. (A.14) in the form

$$b = a_1 \exp(-i\hbar\{\cdot\}/2) a_2 \tag{A.15}$$

When a_1 or a_2 is a polynomial, then sum (A.15) is finite and gives the correct answer. In the general case, Eq. (A.15) represents an asymptotic series, so that it is convenient to write explicitly a finite number of terms in the expansion of the exponential and to exhibit explicitly a remainder, i.e.,

$$b = a_1 a_2 - i(\hbar/2)\{a_1, a_2\} + \cdots + (-i\hbar/2)^N a_1\{\cdot\}^N a_2/(N-1)! + \rho_N \tag{A.16}$$

This is in fact a semiclassical expansion of $b(x, \xi)$ in powers of $\hbar$. Its precise formulation is given by the following.

Theorem A.2. Let $a_1(x, \xi)$ and $a_2(x, \xi)$ be, respectively, two symbols of order m_1 and m_2 and let A_1 and A_2 be the associated operators. Then, the function $b(x, \xi)$ associated with the operator product $B = A_1 A_2$

is a symbol of order m_1+m_2. The remainder ρ_N is a symbol belonging to the class

$$S^{m_1+m_2}(k^N)$$

In order words, one has the following bound for the remainder

$$|\rho_N(x,\xi)| \leqslant K(\hbar/LPM)^N(1+x^2/L^2+\xi^2/P^2)^{-N+(m_1+m_2)/2} \tag{A.17}$$

with similar bounds for its derivatives. The constant K is expressed more precisely by the following rule.

Good-behavior rule. Using microscopic scales of length and momentum ℓ_0 and $\not{p}_0$ such that $\ell_0/\not{p}_0=L/P$ and $\ell_0\not{p}_0=\hbar$, then the constant K occurring in the bound (A.17) is given by

$$K=(c/N!)\sup_{x,\xi,y,n,\alpha,\beta}[\ell_0^{|\alpha|}\not{p}_0^{|\beta|}\,|\,\partial_x^\alpha\partial_\xi^\beta\sigma(\partial_x,\partial_\xi;\partial_y,\partial_n)\,a_1(x,\xi)\,a_2(y,n) \tag{A.18}$$

where c is a numerical constant of order unity depending only upon n and N. The supremum is taken over all the indices α,β such that $0\leqslant|\alpha|+|\beta|\leqslant n+1$.

As a consequence, terms of a given derivative order $|\alpha|+|\beta|$ have also a semiclassical order of magnitude $(\hbar/LP)^{|\alpha|+|\beta|}$, so that generally the leading term is obtained for $\alpha=\beta=0$, i.e.,

$$K\sim(1/N!)\sup_{x,\xi}|a_1\{\cdot\}^N a_2| \tag{A.19}$$

This simple evaluation does not hold when the number of degrees of freedom n becomes very large and when the seminorms of a_1 and a_2 increase rapidly with α and β.

A.3. Norms and Traces

One often needs to put some bounds upon an operator that is given by its symbol. Consider, for instance, a real symbol $a(x,\xi)$ that is known to satisfy the inequalities

$$c_1\leqslant a(x,\xi)\leqslant c_2 \tag{A.20}$$

If one thinks of $a(x,\xi)$ as some classical version of the associated observable A, one is tempted to assume the approximate validity of the inequalities

$$C_1 I\leqslant A\leqslant c_2 I? \tag{A.21}$$

This would give immediately an estimate for the norm of A, namely the supremum of $|c_1|$ and c_2.

This assumption turns out to be true up to corrections of order $(\hbar/LP)^2$. It may be useful to sketch why this happens before stating the precise correct results. Subtracting c_1 or c_2 from $a(x, \xi)$, it is obviously enough to ask which bound for the operator A results from the inequality

$$a(x, \xi) \geqslant 0 \tag{A.22}$$

If the positive square root $b(x, \xi) = [a(x, \xi)]^{1/2}$ is a symbol, one can associate an operator B with it. Theorem 2 can then be used to show that the square of the operator B has a symbol

$$b^2(x, \xi) - (\hbar^2/8)\, b\{\cdot\}^2 b + \cdots$$

where one has used Eq. (A.15). The first term is $a(x, \xi)$ and the associated operator is A. The next term is of order $\hbar^2$ because the first term $\{b, b\}$ is identically zero. This suggests a relation $A = B^2 + A'$, i.e., $A \geqslant A'$, where A' is an operator proportional to $\hbar^2$.

The example $a(x, \xi) = x^2$ shows, however, that in that case $b(x, \xi) = |x|$ is not differentiable, so that due caution must be exercised. The result of a careful and difficult analysis is the so-called "sharp Gärding inequality," which will be given here in a special but useful case.

Theorem A.3. Let $a(x, \xi)$ be a *positive* symbol belonging to $S^0(k^{-2})$. Then one has the inequality

$$\langle u|\, A\, |u\rangle \geqslant -C \tag{A.23}$$

for any normal wave function u belonging to the Schwartz set $\mathscr{S}$ of rapidly decreasing C^∞ functions.

The constant C only depends upon n and is essentially one of the seminorms $C'_{\alpha\beta}$ of a as an element of $S^0(k^{-2})$ as given by the bounds (A.9), i.e.,

$$|\partial_x^\alpha \partial_\xi^\beta a(x, \xi)| \leqslant C'_{\alpha\beta}(LP/\hbar)^2[1 + (x^2/L^2) + (\xi^2/P^2)]^{2-(|\alpha| + |\beta|)/2}$$

Generally, one is interested in a symbol $a(x, \xi)$ satisfying the bounds (A.8) with constants $C_{\alpha\beta}$ of order unity, so that the constants $C'_{\alpha\beta}$ can be taken of order $(\hbar/LP)^2$. If, furthermore, $a(x, \xi)$ is a symbol of order zero, so that A is bounded according to Theorem 1, the inequality (A.234) is valid for any normed wave function u with no differentiability condition upon it. Then it follows that $\langle u|\, A\, |u\rangle$ is larger than a negative constant of order $(\hbar/LP)^2$. This result is extremely useful to bound a spectrum or a norm.

It should be noticed that a positive symbol does not strictly correspond to a positive operator. The reciprocal property is well known in physics, since a positive density operator does not strictly correspond to a positive Wigner distribution function.

Along with the ordinary norm in Hilbert space, two other kinds of norms are useful, namely the Hilbert–Schmidt norm

$$\|\Omega\|_{\mathrm{HS}}^2 = \mathrm{Tr}(\Omega^+\Omega) \tag{A.24}$$

and the trace norm

$$\|\Omega\|_{\mathrm{tr}} = \mathrm{Tr}\,|\Omega| = \mathrm{Tr}(\Omega^+\Omega)^{1/2} \tag{A.25}$$

When $\|\Omega\|_{\mathrm{tr}} < \infty$, the operator Ω is said to be of trace class and its ordinary trace is then well defined independently of the basis in Hilbert space.

The Hilbert–Schmidt norm is easily expressed in terms of the corresponding symbol by

$$\|\Omega\|_{\mathrm{HS}}^2 = \int |\langle x|\,\Omega\,|x\rangle|^2\, dx = \int |\omega(x, \xi)|^2\, dx\, d\xi/(2\pi\hbar)^n \tag{A.26}$$

The trace norm plays a central role in applications to quantum mechanics or statistical mechanics. This is because quantum averages are given by traces and one will often be led to bound such a trace using the inequality

$$|\mathrm{Tr}(AB)| \leqslant \|A\| \cdot \mathrm{Tr}\,|B| \tag{A.27}$$

It is therefore important to get an estimate of $\mathrm{Tr}\,|\Omega|$ from the knowledge of a symbol $\omega(x, \xi)$. Here again, this is a difficult problem with a nontrivial answer and it will be useful to first give a hint about its solution in order to make clearer the answer.

Consider the case of a positive real symbol $a(x, \xi)$ vanishing outside a bounded region D. One can still use formally Theorem A.2 to write $A = B^2 + A'$, where B is the operator with symbol $a(x, \xi)^{1/2}$, assuming that this square root is indeed a symbol, and $a'(x, \xi)$ is a function of order $(\hbar/LP)^2$. Then one can write

$$\mathrm{Tr}\,|A| \leqslant \mathrm{Tr}\,B^2 + \mathrm{Tr}\,|A'| \tag{A.28}$$

Let $c(x, \xi)$ be the symbol of the operator B^2. According to Eq. (A.6), one has

$$\mathrm{Tr}\,B^2 = \int c(x, \xi)\, dx\, d\xi/(2\pi\hbar)^n \tag{A.29}$$

and, according to Theorem 2,

$$c(x, \xi) = b(x, \xi) \exp(-i\hbar\{\cdot\}/2)\, b(x, \xi) \tag{A.30}$$

When Eq. (A.30) is inserted into Eq. (A.29), integration by parts shows that all the terms in the expansion of the exponential give a zero contribution to the integral in Eq. (A.29) except for the leading term, so that one simply gets

$$\operatorname{Tr} B^2 = \int b^2(x, \xi)\, dx\, d\xi/(2\pi\hbar)^n = \int a(x, \xi)\, dx\, d\xi/(2\pi\hbar)^n$$

and one expects $\operatorname{Tr} A'$ to be of order $(\hbar/LP)^2$.

When $a(x, \xi)$ is not positive, one can try to decompose it into a difference $a_+(x, \xi) - a_-(x, \xi)$, where, for instance, $a_+(x, \xi) \geqslant 0$, $a_-(x, \xi) \geqslant 0$. This would suggest that

$$\operatorname{Tr} |A| = \int (|a_+(x, \xi)| + |a_-(x, \xi)|)\, dx\, d\xi/(2\pi\hbar)^n = \|a\|_{L^1}(2\pi\hbar)^{-n}$$

up to corrections of order $(\hbar/LP)^2$. The same property is also expected when $a(x, \xi)$ is a complex quantity. Here $\|a\|_{L^1}$ is the ordinary Lebesgue integral of the absolute value of $a(x, \xi)$. To estimate the corrections and to get the best choice for a_+ and a_- is a highly nontrivial task. The most convenient form of the result for the applications is probably the following one.[14]

Consider the scales ℓ_0 and p_0 such that $\ell_0/L = p_0/P$ and $\ell_0 p_0 = \hbar$ and let B denote the "unit" ball

$$x^2 \ell_0^{-2} + \xi^2 p_0^{-2} \leqslant 1$$

Given a function $a(x, \xi)$, one will denote by $\delta a(x, \xi)$ the function

$$\delta a(x, \xi) = \sup_{(t, \tau) \in B;\, |\alpha| + |\beta| = n+1} |\ell_0^{|\alpha|} \partial_x^\alpha p_0^{|\beta|} \partial_\xi^\beta a(x + t, \xi + \tau)| \tag{A.31}$$

which is typically of order $(\hbar/LP)^{n+1}$. Then one gets the following result.

Theorem A.4. One has the estimate

$$\|A\|_{\mathrm{tr}} \leqslant C_1 \|a\|_{L^1}(2\pi\hbar)^{-n} + C_2 \|\delta a\|_{L^1}(2\pi\hbar)^{-n} \tag{A.32}$$

C_1 and C_2 are constants of order unity.

This last result concludes the list of basic theorems necessary for the applications in the present paper. As a final remark, I shall indicate how they can be used to localize the action of an operator in different regions of classical phase space (hence the name microlocal analysis). One can cover phase space by some cells C^r and introduce a corresponding partition of unity, that is, a family of C^∞ functions $\{\varphi^r(x, \xi)\}$ such that the support of $\varphi^r(x, \xi)$ is essentially C^r and

$$\sum_r \varphi^r(x, \xi) = 1$$

whatever (x, ξ). Given a symbol $a(x, \xi)$, one can write it as a sum

$$a(x, \xi) = \sum_r a_r(x, \xi)$$

where each symbol $a_r(x, \xi) = a(x, \xi)\, \varphi^r(x, \xi)$ is localized (nonzero) in a neighborhood of C^r. Theorem A.2 allows one to replace this elementary partitioning by a property of operators. This powerful localization technique allows the consideration of a general kind of configuration space and not only $\mathbb{R}^n$, i.e., a general kind of phase space and not only $\mathbb{R}^{2n}$.

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