Università di Napoli *Federico II*
Corso di Complementi di Meccanica Quantistica tenuto da Fedele Lizzi

Appunti sulla Quantizzazione dei Sistemi Dinamici

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Nota. I seguenti appunti sono in forma provvisoria e sono ad esclusivo uso interno del corso. Sono in inglese perché tratti in parte da un libro in preparazione con G. Landi e R.J. Szabo.

1 Quantum and Classical Mechanics

Rigorously speaking in nature there exist only (relativistic) quantum mechanical systems, which in some limits behave in a way well modelled by classical mechanics. The classical limit is well studied and understood, even if it is not free of ambiguities, often related to the measurement process. Since our sizes, energies etc. make us experience a word well described by the classical models we are in general more familiar with classical quantities, and define the quantum mechanical ones by analogy. For example quantum position and momenta (operators) and their connection with the analogous quantities on the classical phase space. One of the main differences is that the former *do not commute*, so that the quantum phase space becomes *noncommutative*, and hence not a space in the usual sense! Instead of an ensemble of points we have some operators acting on some Hilbert space, or better an algebra of operators and a set of density matrices. So we need to understand this quantum phase space, and how to obtain it (when and if possible) from the classical one.

At the level of abstract definitions one could easily define the noncommutative algebra of a quantum phase space (at least in the simplest cases) as the one generated by the position and momentum operators acting on a separable Hilbert space. Looking at the algebra of observables, one can even take the point of view of considering all observables (in the sense of Dirac), that is the self-adjoint elements of the huge algebra of all bounded operators on the Hilbert space. Those definitions are however not particularly useful without making a connection with *classical* mechanics, understanding the processes of quantization. This is a very large topic, and we limit ourselves to a choice of some aspects. The bibliography at the end is by no means complete and only suggests some further readings on the subject.

Both quantum and classical mechanics study the evolution in time of physical systems. Their original setting is common, the evolution of systems of point particles, albeit in different regimes and with different levels of approximations. The two theories are, however, fundamentally different, not so much in that in a variety of examples they give different answers, but in that they ask different questions. While classical mechanics is concerned with position, trajectories, and in general with the state of the system in phase space (or in the space of positions and velocities), in the quantum theory the questions asked deal with probabilities, possible results of measurement etc. The connections between the two theories are the problems of quantization and of the classical limit.

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2 The Phase Space in Classical Mechanics

Classical mechanics is naturally a geometric theory. In both its Lagrangian and Hamiltonian versions the natural framework in which to describe it are manifolds and vector bundles. In the Hamiltonian point of view the states of a system are described by the phase space M, a manifold which is the cotangent bundle of the space of configurations (positions) of the particles, or, more generally, a generic manifold in which a *Poisson Bracket* is defined. In all generality a Poisson bracket is a map which gives, for each pair of smooth functions on M, another smooth function on M:

$$\{\cdot,\cdot\} : C^\infty(M) \times C^\infty(M) \to C^\infty(M) \ . \tag{2.1}$$

It is linear in both arguments, antisymmetric, and satisfies the Jacobi identity,

$$0 = \{f, \{g, h\}\} + \{g, \{h, f\}\} + \{h, \{f, g\}\} \ , \tag{2.2}$$

i.e. it defines a Lie bracket on $C^\infty(M)$. In addition it satisfies the Leibnitz rule,

$$\{f, gh\} = g\{f, h\} + \{f, g\}h \ , \tag{2.3}$$

i.e. it is a derivation of $C^\infty(M)$. To give a Poisson bracket is equivalent to the specification of a *Poisson bivector* Λ

$$\{f, g\} = \Lambda(\mathrm{d}f, \mathrm{d}g) \ , \tag{2.4}$$

which in term of local coordinates u^i for M becomes:

$$\{f, g\} = \Lambda^{ij} \frac{\partial f}{\partial u^i} \frac{\partial g}{\partial u^j} \ , \tag{2.5}$$

where (Λ^{ij}) is antisymmetric. Functions on M (possibly with an explicit dependence on time) are the classical observables. Given a *Hamiltonian* function H, their time evolution is given in terms of the Poisson bracket as

$$\frac{\mathrm{d}f}{\mathrm{d}t} = \frac{\partial f}{\partial t} + \{H, f\} \ . \tag{2.6}$$

For an n dimensional configuration space Q, $M = T^*Q$ is the cotangent bundle. We can then define a symplectic structure which is a nondegenerate closed two-form ω, whose inverse is the bivector field Λ. When $Q = \mathbb{R}^n$, then $M = \mathbb{R}^{2n}$ and we can find global coordinates u^i on M for which the antisymmetric matrix (Λ^{ij}) is in its *canonical form**

$$(\Lambda^{ij}) = \begin{pmatrix} 0 & \mathbb{1}_n \\ -\mathbb{1}_n & 0 \end{pmatrix} . \tag{2.7}$$

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These coordinates (called Darboux coordinates) can be interpreted as positions and momenta:

$$q^i = u^i \quad , \; p_i = u^{i+n} \quad , \; i = 1 \dots n \; , \tag{2.8}$$

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and in this case

$$\{f, g\} = \frac{\partial f}{\partial q^i}\frac{\partial g}{\partial p_i} - \frac{\partial f}{\partial p_i}\frac{\partial g}{\partial q^i} \tag{2.9}$$

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3 The Phase Space in Quantum Mechanics

In the quantum mechanics of systems with a finite number of degrees of freedom, positions and momenta become noncommuting operators on a Hilbert space. Because of Heisenberg's uncertainty relation (a direct consequence of the noncommutativity of operators) it is impossible to consider the quantum phase space as a usual geometric object. Now the observables, rather than being functions on a manifold, can be seen as operators on an (infinite dimensional) Hilbert space. A state is no longer a point in phase space, but a vector in the Hilbert space, or rather a density matrix, that can be regarded as a map from (hermitean) operators to real numbers.

In textbooks, quantum mechanical point particle systems are traditionally introduced from the *quantization* of a corresponding classical system for which $M = \mathbb{R}^{2n}$. This is via the correspondence principle, which associates to position and momentum variables operators on the Hilbert space $\mathcal{H} = L^2(Q)$. The correspondence is

$$\begin{aligned} \hat{q}_i &\rightarrow q_i \\ \hat{p}_i &\rightarrow -\mathrm{i}\,\hbar\frac{\partial}{\partial q_i} \end{aligned} \tag{3.10}$$

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where the hat distinguishes the quantum operator from the classical variable†. The well known consequence of this relation is the noncommutativity of position and momentum:

$$[\hat{q}^i, \hat{p}_j] = \mathrm{i}\,\hbar\delta^i_j \; , \tag{3.11}$$

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which in turn leads to Heisenberg uncertainty principle

$$\Delta\hat{q}^i\Delta\hat{p}_j \geq \frac{\hbar}{2}\delta^i_j \; . \tag{3.12}$$

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We are thus forced to a "pointless" geometry. Classical observables are promoted to operators and the Poisson bracket is replaced by a commutator:

$$\{f, g\} \rightarrow -\frac{\mathrm{i}}{\hbar}[\hat{f}, \hat{g}] \tag{3.13}$$

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*When $Q \neq \mathbb{R}^n$ this is only possible locally, chart by chart.

†We will soon abandon this notation when there is no possibility of confusion between the quantum operator and the classical quantity.

4 One parameter groups and Weyl Systems

There is a first problem because both position and momenta are unbounded operators. It is easy to see (Wintner theorem) that if two operators have a constant commutator, at least one of them in unbounded. The proof is simple, if both $\hat{p}$ and $\hat{q}$ were bounded, so would be

$$\hat{q}^n\hat{p} - \hat{p}\hat{q}^n = \mathrm{i}\,\hbar n\hat{q}^{n-1} \ , \tag{4.14}$$

and therefore

$$\hbar n\|\hat{q}\|^{n-1} \leq 2\|\hat{p}\|\,\|\hat{q}\|^n \ , \tag{4.15}$$

which implies

$$\|\hat{p}\|\,\|\hat{q}\| \geq \hbar\frac{n}{2} \tag{4.16}$$

for all values of n, which is impossible if both $\|\hat{p}\|$ and $\|\hat{q}\|$ are finite.

The solution proposed by Weyl is to consider not the operators themselves, but the symmetries they generate: translations in the space of position and momenta. In other words to exponentiate them. Consider then two one parameter groups, i.e. two representations of the abelian group on the Hilbert space by unitary operators:

$$\begin{aligned} U(s)\psi(x) &= \psi(x+s) \\ V(t)\psi(x) &= \mathrm{e}^{\,\mathrm{i}\,xt}\psi(x) \end{aligned} \tag{4.17}$$

a direct calculation shows that

$$U(s)V(t) = \mathrm{e}^{\,\mathrm{i}\,st}V(t)U(s) \tag{4.18}$$ weylpq

To these two representations correspond (by Stone Theorem) two Hermitean operators defined as

$$\begin{aligned} \lim_{s\to 0}\frac{U(s)\psi - \psi}{s} &= \mathrm{i}\,\hat{p}\psi \\ \lim_{t\to 0}\frac{V(t)\psi - \psi}{t} &= \mathrm{i}\,\hat{q}\psi \ . \end{aligned} \tag{4.19}$$

The statement of unboundedness translates into the fact that the above limits are well defined only for a subspaces of the Hilbert space (domain of the operator). It is important to notice that the symmetries of translation in configuration or momentum space are well defined also in classical mechanics as canonical transformations, whose generators are classical positions and momenta.

We can be more general, and consider a general symplectic vector field $\mathcal{S}$, i.e. a vector field on which a symplectic form is defined, as we did at the end of Sect. 2. The *canonical quantization* is then a map U from $\mathcal{S}$ to unitary operators with the property

$$W(X+Y) = \mathrm{e}^{\,\frac{\mathrm{i}}{2}\omega(X,Y)}W(X)W(Y) = \mathrm{e}^{\,-\frac{\mathrm{i}}{2}\omega(X,Y)}W(Y)W(X) \tag{4.20}$$

Sush a set of unitary operators is called a *Weyl system*. If it is possible to divide the symplectic space into a sum of position and momenta space, $\mathcal{S} = \mathcal{S}_{\mathrm{pos}} \oplus \mathcal{S}_{\mathrm{mom}}$, we find as a particular one-dimensional case (4.18).

5 The Weyl and Wigner Correspondences

We now establish a connection between the classical and quantum phase spaces, at least for systems with a well defined classical counterpart. We want to associate to each classical observable an operators on $\mathcal{H}$. This is done by the Weyl map. Starting from the correspondence principle (3.10), an immediate problem to solve is an ordering ambiguity. Consider, for example[‡], the classical function: p^2q. To it there correspond various quantum operators: $\hat{p}^2\hat{q}$, $\hat{p}\hat{q}\hat{p}$, $\hat{q}\hat{p}^2$, or any linear combination of these with coefficients which sum to 1. Another problem is the fact that $\hat{p}$ and $\hat{q}$ are unbounded operators, with the consequent problem of definition of domains. To solve these problems we introduce the unitary operator

$$W(u) = W(\eta,\xi) = \mathrm{e}^{\frac{\mathrm{i}}{2\hbar}(\xi\hat{p}+\eta\hat{q})} , \tag{5.21}$$ defW

for $u = (\eta, \xi) \in \mathbb{R}^2$. This implies the choice of symmetric ordering, and W is well defined over all of $\mathcal{H}$.

From (3.11) and the Baker-Campbell-Hausdorff formula it follows that

$$W(u)W(u') = \mathrm{e}^{\frac{\mathrm{i}}{\hbar}\omega(u,u')}W(u+u') \tag{5.22}$$ defW2

with $\omega(u, u') = \xi\eta' - \eta\xi'$ the symplectic structure. This is therefore a Weyl system.

The W's can be used as a basis to define an operatorial transform Ω, which associates to each function of p and q the operator

$$f(p,q) \to \hat{\Omega}(f)(\hat{p},\hat{q}) = \int \mathrm{d}\xi \mathrm{d}\eta \tilde{f}(\xi,\eta)W(\xi,\eta) , \tag{5.23}$$ Weylmap

where

$$\tilde{f}(\xi,\eta) = \int \frac{\mathrm{d}q\mathrm{d}p}{(2\pi)^2} f(p,q)\, \mathrm{e}^{-\frac{\mathrm{i}}{2}(\eta q+\xi p)} . \tag{5.24}$$

is the Fourier transform of f. Were it not for the hat on p and q in (5.21), the expression (5.23) would just Fourier transform back f, instead it associates an operator to each function on the classical phase space. If the function f is real the corresponding operator will be hermitean. The Weyl map has an inverse, called the Wigner map, which maps an operator F into a function, using the identity

$$\mathrm{Tr}\, \mathrm{e}^{\frac{\mathrm{i}}{\hbar}(\eta\hat{q}+\xi\hat{p})} = \delta(\eta - \xi) \tag{5.25}$$

one gets

$$\Omega^{-1}(F)(p,q) = \int \frac{\mathrm{d}\eta\mathrm{d}\xi}{(2\pi)^2\hbar}\, \mathrm{e}^{-\mathrm{i}(\eta q+\xi p)}\, \mathrm{Tr}\, F\, \mathrm{e}^{\frac{\mathrm{i}}{\hbar}(\xi\hat{p}+\eta\hat{q})} \tag{5.26}$$

Different orderings are possible via the insertion in (5.23) of a "weight" function $w(\xi, \eta)$, easily calculated with the Baker-Campbell-Hausdorff formula. The Weyl ordering described above corresponds to $w = 1$. Normal (Wick) ordering in which $a^\dagger = \hat{p} - \mathrm{i}\,\hat{q}$ is always to the left of a corresponds to $w = \mathrm{e}^{-\frac{1}{4\hbar}(\eta^2+\xi^2)}$. The ordering of $\hat{q}$ to the left of $\hat{p}$ corresponds to $w = \mathrm{e}^{-\mathrm{i}\,\eta\xi/2\hbar}$.

[‡]To avoid the proliferation of indices we consider only the one dimensional case in this section.

6 Wigner Distributions

Wigner made an attempt to perform quantum mechanics in phase space attempting to find the analog of a wave function. The analogy is not perfect but the tecniques is useful all the same. Given a classical function and a quantum mechanical pure state we can express

$$\left\langle \hat{\Omega}(f(p,q)) \right\rangle = \int \mathrm{d}p\,\mathrm{d}q f(p,q) W(p,q) \tag{6.27}$$

where

$$W(p,q) := \frac{1}{2\pi} \int \mathrm{d}y \psi^*(q + \frac{y}{2})\,\mathrm{e}^{\,\mathrm{i}\hat{p}y} \psi(q - \frac{y}{2}) \tag{6.28}$$

The Wigner distribution has the property that

$$\begin{aligned} \int \mathrm{d}pW &= |\psi(q)|^2 \\ \int \mathrm{d}qW &= |\tilde{\psi}(p)|^2 \end{aligned} \tag{6.29}$$

but it is not defined positive, and hence cannot be considered as a probability distribution.

Given a non pure state represented by a density matrix $\rho = \sum_n |\psi_n\rangle \rho_n \langle\psi_n|$ the corresponding Wigner distribution will be

$$W(p,q) = \sum_n \rho_n \frac{1}{2\pi} \int \mathrm{d}y \psi_n^*(q + \frac{y}{2})\,\mathrm{e}^{\,\mathrm{i}\hat{p}y} \psi_n(q - \frac{y}{2}) \tag{6.30}$$

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7 Moyal Quantization and Product

With the Weyl map and its inverse we associate to a classical function on phase space an operator, and viceversa. In other words we map classical *commuting* observables to quantum *noncommuting* ones. The former correspond to an ordinary manifold, while the latter describe, in some sense, a noncommutative space. In this section we will view quantum mechanics as a deformation of classical mechanics, bearing in mind that not every quantum system can be viewed as the quantization of a classical one. Nevertheless classical limits do exist and we will see that for classical systems the corresponding quantum observables can be seen as deformations of the classical ones, driven by the "small" parameter $\hbar$. As we said in section 2 the main characteristic of a classical phase space is that it is a Poisson manifold. Functions on it are multiplied in the usual pointwise way, they form a commutative algebra in the language of subsequent chapters. We now define a new product to describe a quantum system, and it is important that classical physics is recovered, at least in some sense, in the limit $\hbar \to 0$. Given two functions on a classical phase space with the usual Poisson bracket (2.9), taking the commutator of the operators obtained with the Weyl map, and then going back to the classical functions with the Wigner map, the result is not the original Poisson bracket (as it might be expected), but an expression which agrees with the latter only to first order in $\hbar$:

$$\Omega^{-1}\left([\Omega(f),\Omega(g)]\right) = \sum_{k=1}^{\infty}\left(\frac{\mathrm{i}\,\hbar}{2}\right)^{2k+1} f\ (\overleftarrow{\partial}_p\overrightarrow{\partial}_q - \overleftarrow{\partial}_q\overrightarrow{\partial}_p)^{2k+1}\ g \tag{7.31}$$

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where the notation $\overleftarrow{\partial}$ (resp. $\overrightarrow{\partial}$) means that the partial derivative acts on the left (resp. left).

Equation (7.31) suggests the definition of a bracket among functions which should describe quantization. For any phase space with constant Poisson structure Λ, the *Moyal bracket* is defined as:

$$[f,g]_\star := \sum_{k=0}^{\infty}\left(\frac{\mathrm{i}\,\hbar}{2}\right)^{2k+1}\Lambda^{2k+1}(\mathrm{d}f,\mathrm{d}g)\ . \tag{7.32}$$

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Using the Weyl map we can define a new deformed product, which we call[§] the $\star$-product

$$f\star g = \Omega^{-1}(\Omega(f)\Omega(g))\ , \tag{7.33}$$

so that

$$[f,g]_\star = f\star g - \ g\star f\ . \tag{7.34}$$

Using the explicit expression of the Weyl map the explicit differential form of the product is

$$(f\star g)(u) := f(u)\ \exp\left(\frac{\mathrm{i}\,\hbar}{2}\ \overleftarrow{\partial}_i\ \Lambda^{ij}\ \overrightarrow{\partial}_j\right)\ g(u)\ , \tag{7.35}$$

defstar

where u is as in (2.8).

With this deformed product it is possible reformulate time evolution of quantum operators as evolution on classical phase space

$$\frac{\mathrm{d}f}{\mathrm{d}t} = \frac{\partial f}{\partial t} + \frac{i}{\hbar}[f,H]_\star \tag{7.36}$$

8 General $*$ Products

The $\star$ product defined in the previous subsection is intimately tied with the canonical structure (2.7), and in turn with the usual commutation relation (3.11). It provides a way to look at quantum mechanics as a deformation and led to the generic quantization under what is called *deformation quantization*. This is based on a generic deformation of the product of functions on a Poisson manifold M, which to first order in the parameter $\hbar$ has a commutator proportional to the Poisson bracket. In a sense quantum mechanics is seen as a dynamics on a noncommutative space. To a particular classical manifold there can correspond several quantum phase spaces, all of which reduce to the same classical case in the limit of $\hbar\to 0$. The $\star$ -product is but one possible deformation.

[§] It is also called the Grönewold-Moyal-Weyl product.

Deformation quantization of a Poisson manifod consists in finding a deformation of the algebra, with the additional property that to first order the $*$ commutator reduces to the Poisson bracket. The conditions for a well defined associative product are very difficult to satisfy. For instance using the definition (7.35) for a nonconstant Λ tensor would give a nonassociative product. Given a Poisson manifold it is highly nontrivial to prove that it is always possible to find a $*$ product whose commutator reduces, to first order in the deformation parameter, to the Poisson bracket. The problem for a generic Poisson manifold has been solved by Kontsevich who was awarded the Field medal for it. It

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