Lecture 1: Reminder of basics of quantum mechanics and canonical quantization in Hilbert space

Ludwig Faddeev

8 October 1996

After hearing some statements on the nature of quantum theory during last week I decided to start my lecture by presenting a suitable and reasonably natural framework into which QM satisfactorily fits. The framework itself is an abstraction of thoughts and essays of many people. I mention P. Dirac, H. Weyl, J. v. Neumann, I. Segal and G. Mackey. I shall be very cryptic.

A description of physical reality is made in terms of two sets of objects: observables and states. A set of observables A, $B, \ldots$ will be denoted by $\mathfrak{A}$ and states ω, $\mu, \ldots$ by Ω. Each state ω assigns to each observable A its probability distribution $\omega_A(\lambda)$ on a real line. The pairing (mean value)

$$\langle \omega | A \rangle = \int \lambda d\omega_A(\lambda)$$

defines a duality between A and Ω. It is natural to assume the separability (completeness) of states: two observables with equal pairings in all states are equal. This immediately introduces a real linear structure on $\mathfrak{A}$, whereas Ω is a convex set. The next structure is a notion of functional dependence of observables. The observable B is a function $f(A)$ of the observable A if in any state

$$\langle \omega | B \rangle = \int f(\lambda) d\omega_A(\lambda).$$

This definition of a function is rather unwieldy, so a technical assymption is added that A lies in an algebra with product AB such that the notion of function is compatible with this product.

Now comes dynamics: each observable generates a motion of $\mathfrak{A}$, that is a one-parameter group of automorphisms of $\mathfrak{A}$ via the differential equation

$$dA/db = \{B, A\},$$

where $\{\ ,\ \}$ is a bracket, which is necessarily of Lie type and is a derivation of the product

$$\{A, BC\} = \{A, B\}C + B\{A, C\}.$$

This essentially finishes the description of the framework.

Both classical and quantum mechanics fit perfectly in it and give concrete and nonequivalent realizations.

All features of CM are reconstructed as soon as one assumes that $\mathfrak{A}$ is commutative. It follows that $\mathfrak{A}$ can be realized as an algebra of functions on a symplectic manifold (phase space) M: states are normalized measures on the phase space and $\{\ ,\ \}$ is a Poisson bracket, defined by the symplectic structure on it. In particular

$$\omega_A(\lambda) = \int \theta\left(\lambda - f_A(p,q)\right) d\mu_\omega,$$

where $\theta(t)$ is a step function, $f_A(p,q)$ is a function corresponding to observable A and μ_ω is a measure corresponding to the state ω. Pure (extremal) states are defined by atomistic measures concentrated in one point of M. All observables have exact values (zero dispersions) in all pure states.

In the case of QM, the set $\mathfrak{A}$ consists of real elements of a complex associative algebra with involution, which is usually realized as an algebra of linear operators in some complex Hilbert space H. The states are the positive trace class operators with unit trace. The distribution $\omega_A(\lambda)$ is given by

$$\omega_A(\lambda) = \mathrm{tr}\ \left(MP_A(\lambda)\right),$$

where M (density matrix) defines the state and $P_A(\lambda)$ is a special projector function of operator A. The dynamical bracket is defined in terms of product

$$\{A,B\} = (i/\hbar)(AB - BA),$$

where $i = (-1)^{1/2}$ and the normalizing factor $1/\hbar$ here employs the famous Planck constant $\hbar$. Its introduction in this place is necessitated just from dimensional considerations.

The pure states are given by one-dimensional projectors and a given observable is exact (dispersionless) only in pure states, defined by its eigenvectors. This feature, which is reflected in the "uncertainty" inequality

$$\Delta_\omega A \Delta_\omega B \geq (\hbar/2) |\left\langle \omega | \{A,B\} \right\rangle|,$$

where

$$\Delta_\omega A = (\left\langle \omega | (A - \langle \omega | A \rangle)^2 \right\rangle)^{1/2}$$

is the main physical distinction between QM and CM. By no means does it preclude the measurability of observables in QM. Indeed, the collection of eigenstates is enough to characterize any observable. On the contrary, the exactness of observables in all pure states in CM is a kind of unnecessary luxury.

It is instructive to compare the CM and QM on some common playing field. We shall consider the simplest mechanical system with *one degree of freedom*: in other words the phase space is $M = \mathbf{R}^2$, and points in phase space are denoted (p,q). The Hilbert space is

$$\mathcal{H} = L^2(\mathbf{R}) = \{\psi(q) \in \mathbf{C} : \int_{q=-\infty}^{\infty} |\psi(q)|^2 dq < \infty\}.$$

Quantum mechanically we replace the basic observables (*canonical* coordinates) p and q by operators P and Q acting on $\mathcal{H}$: these are defined by

$$(P\psi)(q) = \frac{\hbar}{i}\frac{d}{dq}\psi(q), \tag{1}$$

$$(Q\psi)(q) = q\psi(q); \tag{2}$$

this is the so called *coordinate realization.* An observable A is characterized as an integral operator defined by its *kernel*

$$(A\psi)(q'') = \int_{-\infty}^{\infty} A(q'', q')\psi(q')dq'. \tag{3}$$

Alternatively we may define the observable A by means of its *symbol*, which is a function on the phase space M: the symbol f corresponds to the integral kernel A_f by means of the *Weyl quantization*

$$A_f(q'', q') = \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} f(p, \frac{q''+q'}{2})e^{ip(q''-q')/\hbar}dp. \tag{4}$$

There is no unique way to substitute operators for functions because the function pq is equal to the function qp while the operator PQ does not equal the operator QP: one must choose a prescription for the ordering of the operators. The Weyl quantization corresponds to one choice of ordering, which is to completely symmetrize over the operators P and Q. The Weyl quantization is not a homomorphism from the algebra of functions to the algebra of operators: if one associates the operators A_f and A_g to the functions f and g respectively, one may define the kernel of the product $A_f A_g$ by

$$A_f A_g(q'', q') = \int_{-\infty}^{\infty} A_f(q'', q)A_g(q, q')dq. \tag{5}$$

This corresponds to a product $f \star_\hbar g$ on the algebra of functions which equals

$$f \star_\hbar g = fg + \frac{i\hbar}{2}\{f, g\} + O(\hbar^2), \tag{6}$$

so that

$$(i/\hbar)(f * g - g * f) = \{f, g\} + O(\hbar).$$

We see that both CM and QM can be realized in terms of the same objects (functions) but the structure constants of the main operations (product, Lie bracket) of QM are defined as a series in positive powers of $\hbar$, the zero order term being the structure constants of CM. So we can say that QM is a deformation of CM in the framework described above. The Planck constant is a corresponding deformation parameter. This is for me the most concise formulation of the correspondence principle and explains what is meant by quantization.

Now comes the notion of equivalent deformation and that of stability. Beautiful results, which I learned from A. Lichnerowicz, M. Flato and D. Sternheimer, allow one to say that CM is unstable and that QM is essentially a unique deformation of it into a nonequivalent stable structure. The degeneracy of CM (exactness of pure states) is intimately connected with its instability. So it is only natural that the passage from CM to QM was prompted by the experimental activity of physicists. The stability of QM, on the contrary, shows that an analogous modification of it is less feasible. In this case one has first to modify also all the general framework, as emphasized above.

Now I turn to discussion of dynamics. The goal is to make control of the evolution operator

$$U(t) = e^{-iHt/\hbar},$$

which defines the solution of the dynamical equation

$$\frac{dA(t)}{dt} = \{H, A(t)\}_\hbar, \quad A(t)|_{t=0} = A \tag{7}$$

in the form

$$A(t) = U^{-1}(t) A U(t). \tag{8}$$

From now on we take the normalization $\hbar = 1$.

It is convenient to consider arbitrary initial and final times, so we want to construct the kernel of the evolution operator

$$U = e^{-iH(t''-t')} \tag{9}$$

in terms of the symbol corresponding to the Hamiltonian $h(p, q)$. Because Weyl quantization is not a homomorphism taking the product of functions to the product of operators, one cannot substitute the kernel for the Hamiltonian into the Taylor series for the exponential. Nonetheless if $\triangle$ is a small interval, one may make the approximation

$$U_\triangle = e^{-iH\triangle} \cong 1 - iH\triangle \tag{10}$$

and then if $t'' - t' = N\triangle$ one may approximate

$$e^{-iH(t''-t')} = (U_\triangle)^N. \tag{11}$$

We write the integral kernel for $U_\triangle$ as

$$U_\triangle(q'', q') = \frac{1}{2\pi} \int_{-\infty}^{\infty} dp e^{ip(q''-q')} \Big(1 - ih(p, \frac{q''+q'}{2})\triangle\Big) \tag{12}$$

$$= \frac{1}{2\pi} \int_{-\infty}^{\infty} dp e^{ip(q''-q') - ih(p, \frac{q''+q'}{2})\triangle} + O(\triangle^2).$$

To obtain the integral kernel for $e^{-iH(t''-t')}$ we compose N copies of $U_\triangle$ and integrate over the $N-1$ intermediate variables q_j using (5):

$$U(q'', q'; t''-t') = \int \ldots \int e^{ip_N(q_N - q_{N-1}) + ip_{N-1}(q_{N-1} - q_{N-2}) + \ldots + ip_1(q_1 - q_0)} \times \tag{13}$$

$$e^{-ih(p_N, \frac{q_N + q_{N-1}}{2}) - \ldots - ih(p_1, \frac{q_1+q_0}{2})} \frac{dp_1 dq_1}{2\pi} \ldots \frac{dp_{N-1} dq_{N-1}}{2\pi} \frac{dp_N}{2\pi}.$$

In the limit as N tends to infinity while $q_N - q_{N-1}$ is proportional to $1/N$, we formally obtain an integral over trajectories $(p(t), q(t))$ in phase space:

$$U(q'', q'; t'' - t') = \int \exp i \left\{ \int_{t'}^{t''} (p(t)\dot{q}(t) - h(p(t), q(t)))dt \right\} \prod_t \frac{dp(t)dq(t)}{2\pi}. \tag{14}$$

One recognizes

$$\int_{t'}^{t''} (p(t)\dot{q}(t) - h(p(t), q(t))\, dt \tag{15}$$

as the *action functional*, while $\prod_t \frac{dp(t)dq(t)}{2\pi}$ is the Liouville measure on the space of paths.

A *real polarization* of a symplectic manifold or phase space of dimension $2n$ is a surjective map π to a manifold of dimension n such that the fibres are Lagrangian submanifolds (in other words the fibres are of dimension n and the symplectic form restricts to zero on them). The boundary condition on the trajectories in (14) is that $q(t'') = q', q(t') = q'$ while $p(t'')$ and $p(t')$ are unconstrained. This condition says that when t takes the extremal value t' the endpoint of the path $(p(t), q(t))$ lies in a prescribed fibre $L' \stackrel{\text{def}}{=} \pi^{-1}(q')$ of the real polarization

$$\pi : (p, q) \mapsto q \tag{16}$$

of the phase space, while at the other extremal value $t = t''$ the path lies in a different fibre

$$L'' = \pi^{-1}(q'')$$

of the polarization.

Remark: In our example, a phase space arising from a physical system with one degree of freedom is $\mathbf{R}^2$. Other interesting examples arise where the phase space is S^2. No real polarization exists in those cases. Complex polarization leads to finite dimensional represetnation of the group $O(3)$, so that this phase space corresponds to a spin degree of freedom.

If the Hamiltonian is given by

$$h(p, q) = \frac{1}{2}p^2 + v(q), \tag{17}$$

the change of variables

$$p(t) \mapsto p'(t) = p(t) + \dot{q}(t), \quad q(t) \mapsto q(t) \tag{18}$$

transforms the integrand in (15) to a form in which no terms appear which involve both $p(t)$ and $q(t)$ (in other words these variables separate):

$$p'\dot{q'} - h(p', q') = -\frac{1}{2}(p')^2 + \frac{1}{2}(\dot{q})^2 - v(q) \tag{19}$$

We may then integrate over $p(t)$ (to obtain a constant which is independent of $q(t)$) and recover the more usual form of the action which depends only on $q(t)$:

$$U(q'', q'; t'' - t') = \text{const} \int \exp\{i \int_{t'}^{t''} (\frac{1}{2}\dot{q}^2 - v(q))dt\} \prod_t dq(t) \tag{20}$$

Here what appears is the usual Lagrangian, which depends on q and $\dot{q}$ but not on p. This change of variables thus transforms the formula (14) for the kernel of the time evolution operator U into a path integral over trajectories in *configuration* space (the space of possible values of the position) rather than over trajectories in *phase* space (the space of possible values of position and momentum, whose dimension is twice that of the configuration space). We remark that this method of reducing from paths in phase space to paths in configuration space works only when the action is quadratic in the momentum p. However, more general actions quadratic in p can also be treated by this method: for instance, one may use a general Riemannian metric on the configuration space rather than the flat metric p^2, which simply gives rise to a factor of the Riemannian volume element.

Let us now consider an example where the form of the potential $v(q)$ is given explicitly: the *harmonic oscillator*

$$h(p,q) = \frac{1}{2}p^2 + \frac{1}{2}\omega^2 q^2. \tag{21}$$

We intentionally keep here the frequency parameter ω. This will be instructive when we turn to the free fields, which are nothing but a collection of oscillators with different frequencies. The classical equation of motion corresponding to this Hamiltonian is the equation for simple harmonic motion

$$\frac{d^2}{dt^2}q(t) + \omega^2 q(t) = 0. \tag{22}$$

In the approach to quantization which we have described, one finds that the eigenvectors of the Hamiltonian are defined in terms of certain orthogonal polynomials in q, the Hermite polynomials.

The use of special functions can be avoided if one alternatively considers the *holomorphic* quantization of the harmonic oscillator: this will complement the treatment given in K. Gawedski's lectures. We introduce complex coordinates a and a^* on the phase space, defined by

$$a = \frac{1}{\sqrt{2\omega}}(\omega q + ip) \tag{23}$$

$$a^* = \frac{1}{\sqrt{2\omega}}(\omega q - ip) \tag{24}$$

so that

$$q = \frac{1}{\sqrt{2\omega}}(a^* + a). \tag{25}$$

After quantization, a and a^* become operators $\hat{a}$ and $\hat{a^*}$, which satisfy the commutation relation

$$[\hat{a}, \hat{a^*}] = 1. \tag{26}$$

The Hilbert space $\mathcal{H}$ now consists of entire functions in a^*: it is the closure of the space of polynomials in a^* in the norm

$$(f,g) = \int_{\mathbf{R}^2} \bar{f}(a) g(a^*) e^{-a^* a} \frac{da^* da}{2\pi i}. \tag{27}$$

One finds for instance that the elements

$$\psi_n = \frac{(a^*)^n}{\sqrt{n!}} \tag{28}$$

in $\mathcal{H}$ are orthonormal with respect to the norm $(\cdot, \cdot)$. The operators $\hat{a}$ and $\hat{a^*}$ are represented on $\mathcal{H}$ by

$$\hat{a} f(a^*) = \frac{df(a^*)}{da^*}, \tag{29}$$

$$\hat{a^*} f(a^*) = a^* \cdot f(a^*). \tag{30}$$

The Hamiltonian may be written as

$$H = \omega \hat{a^*} \hat{a}, \tag{31}$$

and it has the ψ_n as eigenvectors: we have

$$H\psi_n = n\omega\psi_n. \tag{32}$$

In particular, we have $\psi_0 = 1$, for which $H\psi_0 = 0$; one thus sees that

$$\psi_n = \frac{(\hat{a^*})^n}{\sqrt{n!}} \psi_0. \tag{33}$$

The operators on $\mathcal{H}$ may be represented by integral kernels $A((a^*)'', a')$, which are analytic functions of two independent variables $(a^*)''$ and a'. The composition of two operators corresponds to the following operation on their kernels A and B:

$$(AB)((a^*)'', a') = \int A((a^*)'', \alpha) B(\alpha, a') e^{-\alpha^* \alpha} \frac{d\alpha^* d\alpha}{2\pi i}. \tag{34}$$

Occasionally we shall drop the primes on a^* and a in cases when this does not lead to confusion.

Another possibility is to use *normal symbols*: if we write the operator A as

$$A = \sum_{n,m} K_{mn} (\hat{a^*})^n \hat{a}^m, \tag{35}$$

then the corresponding normal symbol is

$$K(a^*, a) = \sum_{n,m} K_{mn} (a^*)^n a^m. \tag{36}$$

It is an exercise to see that

$$K(a^*, a) = e^{-a^* a} A(a^*, a). \tag{37}$$

If we now turn to dynamics, the kernel of the evolution operator for a small time interval $\triangle$ may be written in terms of the normal symbol of the Hamiltonian $h(a^*, a)$ as

$$U_\triangle = e^{-a^* a - ih(a^*, a)\triangle}. \tag{38}$$

To write the time evolution operator for the time interval $t'' - t'$, we compose N copies of $U_\triangle$ as before:

$$U(a^*, a) = \int \ldots \int e^{a_N^* a_{N-1} - a_{N-1}^* a_{N-1} + a_{N-1}^* a_{N-2} - \ldots - a_1^* a_1 + a_1^* a_0} \times \tag{39}$$

$$e^{-i\{h(a_N^*,a_{N-1})+\ldots+h(a_1^*,a_0)\}\triangle}\prod_{k=1}^{N-1}\frac{da_k^*da_k}{2\pi i}.$$

In this context the analogue of the condition that q_N and q_0 are fixed is that a_N and a_0 are fixed:

$$a_N = a^*, \quad a_0 = a. \tag{40}$$

In the limit as $N\to\infty$ we obtain

$$U = \int \exp\left\{a^*a|_{t=t''} + \int_{t'}^{t''}\{-a^*\dot{a} - ih(a^*,a)\}dt\right\}\prod_{t'\le t\le t''}\frac{da^*(t)da(t)}{2\pi i}. \tag{41}$$

For values of t that are not equal to the extremal values t' and t'', we assume that $a^*(t) = \overline{a(t)}$, but we do *not* assume this on the boundary: thus we impose the condition that $a^*(t'') = a^* \in \mathbf{C}$ (this is the value that was denoted by a^* in (40)) and similarly $a^*(t) = a \in \mathbf{C}$ (this is the value that was denoted by a in (40)). The variables a^*, a are the arguments of the integral kernel in (39): they are arbitrary complex numbers, in particular we do *not* assume that $a^* = \overline{a}$.

If one now substitutes $h = \omega a^* a$, the integral is Gaussian; using the equations of motion

$$\dot{a} + i\omega a = 0, \quad \dot{a}^* - i\omega a^* = 0 \tag{42}$$

with the boundary conditions $a_N = a^*$, $a_0 = a$ (where a^* and a are arbitrary complex numbers which are not required to be complex conjugate) we then see that

$$a(t) = ae^{-i\omega(t-t')}, \tag{43}$$

$$a^*(t) = a^*e^{i\omega(t-t')}. \tag{44}$$

Note that $a(t)$ and $a^*(t)$ are not complex conjugates of each other. Substituting in (41) we obtain

$$U_0(a^*, a, t''-t') = \exp\left\{ia^*ae^{-i\omega(t''-t')}\right\}. \tag{45}$$

Applying this to an element ϕ of $\mathcal{H}$, we find

$$(U_0\phi)(a^*) = \int \exp\left(a^*\alpha e^{-i\omega(t''-t')}\right)\phi(\alpha^*)e^{-\alpha^*\alpha}\frac{d\alpha d\alpha^*}{2\pi i} \tag{46}$$

$$= \phi(e^{-i\omega t}a^*).$$

This shows that the evolution operator is obtained by simply substituting the same argument rotated *backward* in time.