

# Lecture 2: Elements of the History of Quantum Mechanics II

## 1 Birth of Quantum Mechanics 3: Born, Heisenberg, Jordan

We mentioned in chapter “[Lecture 1: Elements of the History of Quantum Mechanics I](#)” that a line of research was centered on finding relations between the structure of the energy levels and the frequency of the emitted radiation and on describing the scattering from a dipole. A preliminary theoretical analysis of the polarization problem was done by van Velt [3, 23].

Later Born [2] made a more detailed study with the purpose of *presenting the results in a form that may give suggestions on how to make the transition from Classical Mechanics to a New Mechanics*. In this paper Born notices that a completely integrable system (such as the Coulomb system) when presented in action-angle variables *appears as a system of harmonic oscillators*. By means of perturbation theory (developed by Hamilton) this description can be carried over to the same system in interaction with the electromagnetic field. If one describes these *virtual oscillators* according to Bohr’s rules, their frequencies must satisfy

$$\nu(n, n') = \frac{1}{h} [E(n) - E(n')] \quad (1)$$

where  $h$  is Planck’s constant and  $E(n)$  is the energy of the  $n$ th state.

At the conclusions of this fundamental paper Born outlines the guiding lines of the search for a new mechanics and predicts that in this new mechanics finite difference equations will substitute the ordinary differential equations of the old mechanics. Strictly speaking Born’s suggestion proved to be incorrect, but a trace of *finite difference scheme* can be seen in the formulation of the theory in terms of Hilbert space operators (infinite matrices).

Bohr’s correspondence principle states that if  $k$  and  $n$  are very large and  $\frac{|k-n|}{k}$  is very small, formula (Eq.(13) in chapter “[Lecture 1: Elements of the History of Quantum Mechanics I](#)”) for the frequency of the radiation emitted or absorbed in the transition between atomic levels must have a classical analogue [1, 3]. According to

Bohr's correspondence principle the parameters should be determined by comparison with the classical theory.

Each stationary state  $\sigma_n$  of the atom is regarded by Born as *equivalent* to a collection of harmonic oscillators (virtual resonators) with frequency  $\nu_{n;m}$ ,  $m \in \mathcal{N}$ . One has  $\nu_{n;m} = K |\nu_n - \nu_m|$  with a universal constant  $K$ . Remark that harmonics do not appear in general because  $\frac{E_n - E_m}{E_n - E_h}$ ,  $k \neq m$  are not in general rational numbers. This avoids in perturbation theory the problem of the *small denominators* that makes perturbation analysis difficult in Classical Hamiltonian Mechanics.

The interaction with an electromagnetic field results in a change in frequencies in the oscillators.

It is convenient at this point to recall some elements of the description in classical mechanics of the interaction between an electric dipole and the electromagnetic field, of which Eq. (14) is an approximation in the case of damped harmonic oscillator. The problem can be stated as follows. A completely integrable system with  $N$  degrees of freedom is described in action-angle variables by a hamiltonian  $H_0 = F(J)$  where  $J \equiv \{J_1, \dots, J_N\}$  are the action variables. We denote by  $\theta_k$ ,  $k = 1, \dots, N$  the corresponding angular variables.

We set

$$\omega_k = \frac{1}{2\pi} |\nu_k|, \quad \nu_k = \frac{\partial H_0}{\partial J_k} \quad (2)$$

In hamiltonian mechanics the interaction of an electric dipole with the electric field is described by an interaction hamiltonian  $H^{int} \equiv P \cdot E(t)$ ,  $P \in R^3$ , where  $P$  is the total momentum of the system and  $E(t)$  is the electric field. We denote by

$$P_0 = \sum_{k_i \in \mathcal{N}, i=1, \dots, N} A_{k_1, \dots, k_N}(J) e^{2i\pi(k_1\omega_1 + \dots + k_N\omega_N)} \quad (3)$$

the electric dipole of the unperturbed system.

We assume that the field is weak (in order to apply perturbation theory) and express this by multiplying the interaction term by a small factor  $\epsilon$  to keep track of the order of approximation. The interaction hamiltonian is then

$$H^{int} = \epsilon P_0 \cdot E(t) = \epsilon \sum_{k_i} E(t) \cdot A_{k_1, \dots, k_N}(J) e^{2i\pi(\omega_1 k_1 + \dots + \omega_N k_N)} \quad (4)$$

To determine (to first order in perturbation theory) the dipole momentum of the system one performs a canonical transformation  $J_k, \theta_k \rightarrow J_k^\epsilon, \theta_k^\epsilon$  chosen so that the total hamiltonian  $H^\epsilon \equiv H_0 + \epsilon H^{int}$  is written in the new canonical variables as

$$H_0(J) + \epsilon H^{int}(J, \theta) = H_\epsilon(J^\epsilon) + \epsilon^2 K(J^\epsilon, \theta^\epsilon, \epsilon) \quad (5)$$

where  $K$  is a suitable function, which is assumed to be regular.

By Hamilton's perturbation theory the function  $H^\epsilon$  in the new canonical variables takes the form

$$H^\epsilon(J^\epsilon \cdot \theta^\epsilon) = H_0(J^\epsilon) + E \cdot p_1(J^\epsilon) + E \cdot p_0(J^\epsilon) + O(\epsilon^2) \quad (6)$$

where for each (small) value of  $\epsilon$ ,  $J^\epsilon \equiv \{J_1^\epsilon, \dots, J_N^\epsilon\}$  are a new system of variables in involution and  $p_0(J^\epsilon)$  is the average of  $p_0$  over the angles  $\theta_k$ . Notice that  $H^\epsilon$  in (6) depends on  $\theta^\epsilon$  at order  $\epsilon^2$  only.

The term  $E \cdot p_1(J^\epsilon) + E \cdot p_0(J^\epsilon)$  represent the effective energy of the system (to first order in  $\epsilon$ ) and therefore

$$p_1(J^\epsilon) + p_0(J^\epsilon) \quad (7)$$

is the *effective electric dipole* of the system (to first order in  $\epsilon$ ). Notice that (6) describes the system in term of *adiabatic invariants* (the action variables).

If  $E(t)$  is mono-cromatic with frequency  $\nu_0$  the average of the function  $H(J, \theta)$  over the torus is zero. The canonical transformation which produces (6) is obtained through a generating function  $S(\theta, J^\epsilon, \epsilon)$  by setting

$$\theta_k^\epsilon \equiv \frac{\partial S}{\partial J_k}, \quad J_k^\epsilon \equiv \frac{\partial S}{\partial \theta^k} \quad (8)$$

The function  $S$  is a solution of the Hamilton-Jacobi equation to first order in  $\epsilon$ . The new momentum is to first order in  $\epsilon$

$$p_0 + \epsilon p_1; \quad p_1 = \sum_k \left[ \frac{\partial p_0}{\partial J_k} \frac{\partial S}{\partial \omega_k} - \frac{\partial p_0}{\partial \omega_k} \frac{\partial S}{\partial J_k} \right] \quad (9)$$

Using (8), (9)

$$p_1 = -E \cos 2\pi\nu_0 t \sum_k \sum_{\nu \cdot \tau > 0} \tau_k \frac{\partial}{\partial J_k} \left( \frac{2|A_\tau|^2 \nu \cdot \tau}{(\nu \cdot \tau)^2 - \nu_0^2} \right) \quad (10)$$

where  $\nu^k = \frac{\partial H_0}{\partial J^k}$  are the frequencies of the oscillators (for each value of  $k$  the index  $\tau_k$  runs over the integers).

A hint on the structure of the *new mechanics* should be obtained comparing (10) with the empirical formula obtained by Kramers.

By construction the sequence  $\{E_n\}$  is increasing and has a limit which we conventionally take to be zero (it is the ionization threshold). For  $n$  large and  $n - m$  of order one  $E_m - E_n$  is *infinitesimal* with respect to  $E_n$ . The correspondence principle states that near the ionization threshold the quantum laws should be comparable to the classical laws. Therefore the parameters should be chosen through a comparison of (10) with Kramer's empirical formula [17].

The correspondence rule that emerges by the analysis by Born is

$$\nu \cdot \tau \rightarrow \nu_{n,m}, \quad J \rightarrow nh \quad (11)$$

The second arrow in (11) is Bohr's correspondence principle.

To understand better the role of the first arrow notice that one can envisage an artificial adiabatic process under which the system goes from the state  $n$  to the state  $m$  through (fictitious) very small intermediate steps. One has then

$$\nu \cdot \tau = \sum_k \frac{\partial H_0}{\partial J_k} \tau_k \simeq \frac{1}{h} \sum_k \frac{\partial H_0}{\partial J_k} \frac{\partial J_k}{\partial \mu} = \frac{1}{h} \frac{\partial H_0}{\partial \mu} \quad (12)$$

This approximation is better justified if  $\mu$  is small and therefore if  $n - m$  is of order of magnitude  $\alpha h$  where  $\alpha$  is very small.

On the other hand, by Einstein's rule, if  $m = n + \tau$  one has

$$\nu_{m,n} = \frac{1}{h} |E(n + \tau) - E(n)| \quad (13)$$

Comparing (12) with (13) one sees that the operation performed in passing from the classical rules to the quantum ones consists in *substituting differentials with finite difference quotients* (the finite differences being of order  $h$ ). This allows the use of the correspondence principle to obtain a relation between the classical and quantum coefficients.

Consider the case  $\frac{\tau}{n} \ll 1$ . Then

$$\sum_k \tau_k \frac{\partial \Phi}{\partial J_k} \rightarrow \int_0^1 d\mu \sum_k \tau_k \frac{\partial \Phi}{\partial J_k} \quad (14)$$

From Bohr's quantization rule, if  $\frac{\tau}{n}$  is sufficiently small (and therefore  $\frac{\tau h}{J}$  sufficiently small) one can consider  $\tau_k d\mu \simeq dJ_k$  and therefore

$$\int_0^1 \sum_k \frac{\partial \Phi}{\partial J_k} \tau_k d\mu \simeq \int_0^1 \sum_k \frac{\partial \Phi}{\partial J_k} dJ_k = \frac{1}{h} (\Phi(n + \tau) - \Phi(n)) \quad (15)$$

This identification must hold for any quantum observable in the limit  $\frac{\tau}{n} \rightarrow 0$ . Moreover, since  $|A_\tau(J)|^2 = A_\tau(J) A_{-\tau}(J)$  and  $A_{-\tau}(J) = A_\tau^*(J)$  one must have

$$|A_\tau(J)|^2 \equiv \Gamma(n, m) = \Gamma(m, n), \quad m = n + \tau \quad (16)$$

Performing in (10) the substitutions indicated in (13)–(15) and recalling the definition of  $\Gamma$  in (16) one obtains

$$p_1 = E \cos(2\pi\nu_0 t) \frac{1}{h} \sum_{\tau_k > 0} \left[ \frac{2\Gamma(n + \tau, n)\nu_{n+\tau, n}}{\nu_{n+\tau, n}^2 - \nu_0^2} - \frac{2\Gamma_{n, n-\tau}\nu_{n, n-\tau}}{\nu_{n, n-\tau}^2 - \nu_0^2} \right] \quad (17)$$

This expression must be compared with Kramer's empirical rule (Eq.(16) in Lecture 1). There is a fair agreement if one chooses

$$-\frac{e^2}{4\pi^2 m} f_{n, m} = \frac{1}{h} 2\Gamma(n, m)\nu_{n, m}, \quad \Gamma(n, m) \equiv |A_{m-n}|^2 \quad (18)$$

It follows from (18) that the knowledge of the emission and absorption frequencies *is not sufficient* to determine the matrix elements  $A_{n, m}$ . Only their absolute values are determined; to determine the phases it is necessary to go further in the order of approximation or to study a problem in which the coupling to the electric field has a different expression (e.g. Heisenberg approximated the atom by an anharmonic oscillator).

Recall that  $A_\tau(J)$  are the elements of the series expansion of the momenta  $p_k$  as functions of the angles  $\theta_k$ . Therefore in accordance with Kramers's formula in quantum mechanics the momentum is represented by a quantity which *depends on two indices*  $m$  and  $n$ , namely *by a matrix*. When  $m_k = n_k + h\tau_k$  and  $\tau_k$  is small with respect to  $n_k$  the quantity  $A_{n+h\tau_k, n}$  plays the role of  $A_\tau(J)$  in the classical case, where  $J$  is the set of action variables associated to the state  $n$ .

## 2 Birth of Quantum Mechanics 4. Heisenberg and the Algebra of Matrices

The next step in the construction of the new mechanics was taken by W. Heisenberg. He analyzed the connections among the quantities of type  $A_{n, m}$  associated to classical quantities other than momentum. These could be obtained studying other types of interactions with the electromagnetic field e.g. making use of interactions in which the classical form of the interaction hamiltonian is of the type  $x \cdot E$  (e.g. the formulas for the polarization in a slowly varying electric field).

In this way one can determine the matrices which the new mechanics associates to the observable position and more generally to observables that in hamiltonian mechanics are described by polynomials in the canonical variables position and momentum.

Heisenberg [10] did a detailed analysis of the corresponding formulas and in particular of those that refer to the anomalous Zeeman effect, which is described in classical theory by the equation  $\ddot{x} = -\omega^2 x - \epsilon x^4$ . This led to establish the following correspondence (to the left the classical case, to the right the quantum case)

$$\begin{aligned} \nu(n\tau) \equiv \tau\nu(n) \equiv \tau \frac{1}{h} \frac{\partial E}{\partial n} &\rightarrow \nu_{n, n-\tau} = \frac{1}{h} (E(n) - E(n-\tau)) \\ \nu_{n, \tau_1} + \nu_{n, \tau_2} = \nu_{n, \tau_1 + \tau_2} &\rightarrow \nu_{n, n-\tau} + \nu_{n-\tau, n-\tau-\tau_1} = \nu_{n, n-\tau-\tau_1} \end{aligned} \quad (19)$$

On this basis Heisenberg stated that the correspondence

$$a_\tau(n) e^{it(\omega(n)\cdot\tau)} \rightarrow A_{n,n-\tau} e^{it\omega(n,n-\tau)} \quad (20)$$

holds for any classical observable  $a$  which can be expressed in the form  $a = \sum_\tau a_\tau(n) e^{it(\omega(n)\cdot\tau)}$ .

Heisenberg found the following relation between the quantum representatives  $\hat{a}, \hat{b}$  of the classical observables  $a, b$

$$\hat{b}_{n,n-\tau} = \sum_\alpha \hat{a}_{n,n-\alpha} \hat{a}_{n-\alpha,n-\tau} \quad (21)$$

This is to be compared to the classical case

$$(a^2)(n, t) = \sum_\alpha a_\beta^2(n) e^{it(\omega(n)\cdot\beta)} = \sum_{\alpha,\beta} a_\alpha(n) a_{\beta-\alpha}(n) e^{it[(\omega(n)\cdot\alpha) + (\omega(n)\cdot(\beta-\alpha))]} \quad (22)$$

Remark that (21) is the product rule for matrices, extended to the case of matrices of infinite rank.

This analysis was summarized in two papers by Born and Jordan [4] and by Born et al. [5]. The latter paper is nicknamed *the three men's work*. In this paper the Authors state that, rather than adapting the formalism of Classical Mechanics in an artificial way, *an organic description of a new theory is established* and a mathematically coherent theory is presented which *describes the properties which is characteristic of quantum phenomena and at the same time shows a remarkable analogy with Classical Mechanics*.

In this [5] the Authors speak for the first time explicitly of a *symbolic quantum geometry* which tends for small values of  $h$  to the *visualizable geometry of Classical Mechanics*. The Authors also speak of *relations among observables* and state that any observable *can be represented by an infinite matrix* (i.e. a linear operator in an infinite dimensional Hilbert space). The Authors stress that these matrices are not of the same type as those which Hilbert was studying in the same years (at that time both the Authors and D. Hilbert were working in Göttingen). The operators that Hilbert was studying are now called Hilbert-Schmidt operators; we will verify that the operators which represent position and momentum *cannot be of Hilbert-Schmidt type*.

In [4, 5] the Authors develop the quantum matrix calculus, establish perturbation theory in Quantum Mechanics (in strict analogy with hamiltonian perturbation theory) and develop in detail the formalism up to second order. The example treated in more detail is that of the anharmonic oscillator with a fourth order anharmonic term. The results were in good agreement with experimental data. It is curious to observe that in this case the perturbation series does not converge. The series is however asymptotic, therefore for small perturbations the analysis to second order gives a satisfactory answer.

The contents of these important papers establish *the essential part* of the present day algebraic-axiomatic formulation of Quantum Mechanics. One can evidence

- the use of methods of *symbolic differentiation* that (in a present days language) substitutes the vector field of Classical Mechanics with the algebraic expression *commutator of two matrices*. In this respect a special role is taken by the matrices  $\hat{q}_k, \hat{p}_k$  which are associated to the coordinates in phase space.
- the writing of the equations in the form

$$\frac{d\hat{q}_k}{dt} = i[\hat{H}, \hat{q}_k] \quad \frac{d\hat{p}_k}{dt} = i[\hat{H}, \hat{p}_k] \quad k = 1, \dots, N \quad (23)$$

where the matrix  $\hat{H}$  describes the interactions present in the system and  $N$  is the number of degrees of freedom of the classical system.

- the proof that the Eq. (23) are (formally) variational equation for the functional

$$\int [(\hat{p}, \hat{q}) - \hat{H}(\hat{q}, \hat{p})] dq dp \quad q = \{q_1, \dots, q_N\} \quad p = \{p_1, \dots, p_N\}$$

(if the definition of integral is properly interpreted).

- the *demonstration* that the quantum counterpart of

$$1 = 2\pi \sum_{\tau} \{q_{\tau}^h, p_{\tau}^h\}, \quad p_{\tau}^h \equiv \nabla_{\tau}(q_{\tau}^k) \quad (24)$$

(where  $\{q, p\}$  denotes Poisson brackets) is the identity

$$[\hat{p}_k, \hat{q}_h] = \frac{h}{2i\pi} \delta_{k,h} I \quad (25)$$

where  $I$  is the (infinite dimensional) identity matrix.

Still it should be remarked that the other identities

$$[\hat{p}_k, \hat{p}_h] = [\hat{q}_k, \hat{q}_h] = 0, \quad k \neq h \quad (26)$$

is postulated by Born, Heisenberg and Jordan without strictly convincing arguments.

From this brief analysis it is clear that in the new mechanics a special role is reserved to infinite matrices  $\hat{q}_k, \hat{p}_h$  which satisfy, at least formally, the commutation relations

$$[\hat{q}_k, \hat{p}_h] = i\hbar \delta_{h,k} I, \quad h, k = 1 \dots N \quad \hbar = \frac{h}{2\pi} \quad (27)$$

all other commutators being set equal to zero.

Notice that in view of (27) the matrices that appear in quantum mechanics are complex valued. We shall see that the natural space for their action is the linear space of sequences of complex numbers  $\phi \equiv \{c_{n,m}, m \in \mathbb{Z}\}$  such that  $\sum_{m=1}^{\infty} |c_{n,m}|^2 = 1$ .

From (2) follow Heisenberg's *uncertainty relations* i.e. that there is no basis in which the matrices  $\hat{q}_k$  and  $\hat{p}_k$  can be simultaneously diagonalized (we shall see later a more precise statement).

Later we shall see that the context of the theory led to interpret  $|c_k|^2$  as the probability that system be in the  $k$ th (atomic) state.

It follows that  $\sum |c_k|^2 = 1$ . If one endows the linear space with the scalar product

$$(\phi^1, \phi^2) \equiv \sum_k (c_k^1)^* c_k^2 \quad (28)$$

the space becomes the Hilbert space  $l^2(N)$ .

We shall see that in order to represent observable quantities the matrices must have real eigenvalues. This forces these matrices to be hermitian. In fact a stronger requirement must be satisfied, i.e. acting on  $l^2(N)$  they must be self-adjoint (in the course of these lecture we will explain the difference).

A relevant contribution to the success of the new Quantum Mechanics was the analysis made by Pauli [20] of the spectrum of the Hydrogen atom using only the algebraic rules of matrix mechanics, i.e. only the commutation relations between the operators (matrices) obtained by using the algebraic rules for the generators of the rotation group and the Runge-Lenz vector (which are constants of motion) for fixed values of the hamiltonian. We shall sketch the analysis of Pauli at the end of this lecture and give more details in chapter "[Lecture 18: Weyl's Criterium, Hydrogen and Helium Atoms](#)".

The analogy of the new formalism with hamiltonian Dynamics permits also a description in the new theory of the interactions of particles in space, in particular scattering. In the same way as Pauli did for the hydrogen atom one can use the algebraic rules of matrix mechanics to describe Rutherford's scattering by an atomic nucleus.

### 3 Birth of Quantum Mechanics 5. Born's Postulate

A very important step in the formulation of Quantum Mechanics was taken by M. Born. He noticed that all waves corresponding to atomic states were square integrable while in classical mechanics one has integrability of the (real valued) distribution of charge, masses etc.

This suggests that  $|\phi(x)|^2$  have a role similar to density. Since the particle is not a fluid Max Born assumed that the real positive function  $|\phi(x)|^2$  represents a density of probability i.e. a *probability density*.



In particular, if one performs a measurement of position,  $\int_{\Omega} |\phi(x)|^2 dx$  is the probability that the particle be found in  $\Omega$ . It follows that

$$\int_{R^3} F(x) |\phi(x)|^2 dx \quad (29)$$

gives the average of the results that are obtained measuring the observable  $F(x)$  in a state described by  $\phi$ .

In the same way, according to Born, if  $\hat{\phi}(p)$  is the Fourier transform of  $\phi$ , the quantity  $|\hat{\phi}(p)|^2$  represents the probability density that, if one measures the momentum of the particle, the integral

$$\int_{R^3} G(p) |\hat{\phi}(p)|^2 dp \quad (30)$$

gives the average result that one obtains making a measurement of the observable  $G(p)$  in a state described by  $\phi$ .

In the Hilbert space terminology, Born's postulate takes the form

$$\bar{F}_{\phi} = (\phi, F(x)\phi), \quad \bar{G}_{\phi} = (\hat{\phi}, G(\hat{p})\hat{\phi}) \quad (31)$$

and can be extended to any other quantum observable if one were able to associate to any observable  $a$  an operator  $A$ . The mean value of  $a$  in the state  $\phi$  will then be  $\bar{a}_{\phi} = (\phi, A\phi)$ . In order to obtain real numbers the operator  $A$  must be symmetric.

## 4 Birth of Quantum Mechanics 6. Pauli; Spin, Statistics

Returning now to Schrödinger's formulation of Quantum Mechanics we remark the solution to evolution equation

$$i\hbar \frac{\partial \phi}{\partial t} = H\phi \quad (32)$$

where  $\phi$  belongs to a complex Hilbert space  $\mathcal{H}$  and  $H$  is a suitable operator (at least formally)

$$\phi(t) = e^{-i\frac{t}{\hbar}H} \phi(0) \quad (33)$$

By Born's postulate the map  $\phi(0) \rightarrow \phi(t)$  must be unitary and this implies that the operator  $H$  is self-adjoint (we will explain later the difference between "self-adjoint" and "closed and symmetric"; in the finite-dimensional case there is no difference).

Moreover Born's postulate implies the wave functions that differ by a constant phase represent the same state. This property implies that symmetries of the system

under a group  $\mathcal{G}$  of transformations are described by *projective representations* of  $\mathcal{G}$  in the Hilbert space. An important example is symmetry under rotations and the introduction of the *spin*.

To account for the hyperfine structure of the spectrum of the atoms, in particular of the helium atom, Pauli [15, 16] *postulated* the existence of particles of *spin*  $\frac{1}{2}$ , introducing thereby *the spin*, a quantity extraneous to Classical Mechanics.

The wave function of a particles of *spin*  $\frac{1}{2}$  transforms under rotations according to a faithful representation of the  $SU_2$  group (which is a double covering of the rotation group) acting in a two-dimensional complex Hilbert space. This is a projective representation of the rotation group. It is by definition a *spinor*. The name *spin* is somewhat connected with spinning, i.e. set something in rotation. The notation  $\frac{1}{2}$  has its origin in the fact that the product of two two-dimensional representations of  $SU_2$  contains the (real) vector representation of the rotation group which corresponds to angular momentum one. Therefore in some sense these particles have half unit of angular momentum.

The presence of spin doubles the number of atomic levels, and the coupling of spin degree of freedom with the magnetic field accounts for a small difference in energy between the two levels in a pair, i.e. for the *hyperfine structure* of the emission lines.

The doubling of the number of degrees of freedom has an another important consequence.

Consider

$$\mathcal{H} \equiv L^2(R^3) \times C^2, \quad \Phi \in \mathcal{H} \equiv \{\phi_1, \phi_2\} \quad \phi_i \in L^2(R^3) \quad (34)$$

as a Hilbert space with scalar product

$$(\phi_k, \phi_h) = \int \bar{\phi}_k(x) \cdot \phi_h(x) dx \quad k, h = 1, 2 \quad (35)$$

In this space which is isomorphic to  $L^2(R) \otimes C^2$  one can define, following Pauli, a first order differential operator  $\tilde{\nabla}$  whose “square” is minus the Laplacian times the identity. It is defined by the matrix-value differential operator

$$\tilde{\nabla} \Phi = \sum_{h=1}^3 \sigma_h \nabla \Phi \quad (36)$$

where the  $2 \times 2$  hermitian matrices  $\sigma_i$  (Pauli matrices) are such that

$$[\sigma_k \sigma_h] = i \epsilon_{k,h,j} \sigma_j, \quad k, h, j = 1, 2, 3 \quad (37)$$

Here  $\epsilon$  is the Ricci symbol, taking value zero if two of the indices are equal, plus one if the permutation is even and minus one if the permutation is odd. One has  $Tr(\sigma_k) = 0 \quad \forall k$  (the matrices  $\sigma_k$  have trace zero).

It is also easy to verify that

$$(\tilde{\nabla})^* \tilde{\nabla} = -\Delta \times I \quad (38)$$

Therefore the operator  $\tilde{\nabla}$  deserves the name of “square root” of minus the Laplacian (notice that the Laplacian is a negative operator as one sees taking Fourier transforms).

Notice now that from (38) it follows that the solution of the equation

$$i \frac{\partial \Phi(t, x)}{\partial t} = (-\Delta \times I) \Phi(t, x) \quad \phi \in L^2(R^3) \otimes C^2 \quad (39)$$

is a spinor with components *that satisfy the free Schrödinger equation*.

In the interacting case, one distinguishes between interaction with the electromagnetic field and other type of interactions. As in the classical case, the interaction with the electromagnetic field is described by adding a vector potential  $A$  to the momentum and a scalar term (electrostatic potential) to the potential.

In the Schrödinger equation this results in substituting  $i\tilde{\nabla}$  with  $i\tilde{\nabla} - A(t, x) \times I$  (recall that  $i\nabla$  is a symmetric operator) and adding a term  $U(t, x)$  to the interaction potential.

Therefore Eq. (39) becomes

$$i \frac{\partial \Phi}{\partial t} = (i\tilde{\nabla} + A \times I)^2 \Phi(t, x) + V(x) \Phi(t, x) \quad (40)$$

for some potential  $V$  (that includes the electrostatic potential).

Another very important consequence of the fact that wave function which differ only by a constant phase represent the same state is the possibility to introduce the *statistics of identical particles*. The (elementary) particles are subdivided in two distinct categories: that of *bosons* for which the permutation of the indices of identical particles does not alter the wave function (Bose-Einstein statistics) and that of *fermions* in which this operation multiplies the wave function by a factor  $-1$  (Fermi-Dirac statistics).

It follows that the wave function of a state which describes two identical fermions cannot be the product of the corresponding wave function: two fermions cannot be in the same state (Pauli *exclusion principle*) [16]. This is at the basis of the properties of the spectra of atoms and molecules and is also responsible for the *stability of matter*.

To the contrary the wave function  $\psi(x_1, \dots, x_N)$  of any number of bosons may be the product of the same wave function, i.e.

$$\psi(x_1, \dots, x_N) = \phi(x_1) \cdots \phi(x_N) \quad (41)$$

i.e. two identical bosons are allowed to occupy the same state.

This is at the root of the properties of the black-body radiations if one assumes that the photons satisfy the Bose-Einstein statistics; it also at the root of the *Bose-Einstein condensation*, a phenomenon predicted by Bose and Einstein and observed experimentally only in recent years.

The ability to account in a simple way for phenomena which don't have a classical counterpart has contributed to the success of Quantum Mechanics.

Notice that *it is a matter of fact* that in nature the wave function of a bosons transform under rotation according to a representation of the rotation group while the wave function of a fermion transforms according to a representation of  $SU(2)$ .

Notice that there is a strict correspondence between the symmetry properties under exchange of indices and the behavior under the rotation group. This fact has *no explanation* within non-relativistic Quantum Mechanics although it is true that only in the case of particles with spin  $\frac{1}{2}$  one is naturally led to use a Hilbert space that admits a non-trivial representation of the permutation group. In the relativistic Quantum Field Theory the connection between spin and statistics is a consequence of locality and positivity of energy.

## 5 Further Developments: Dirac, Heisenberg, Pauli, Jordan, von Neumann

Soon after the proposals of Wave Mechanics by Schrödinger and of matrix mechanics by Born, Heisenberg and Jordan, the *equivalence*, at least at a formal level, of the two formulations was noticed by Schrödinger [21], Eckart [9], Jordan [13], Lademburg [18], Pauli [19], Dirac [6].

It is indeed easy to verify that the canonical commutation relations (27) are satisfied (at least formally) by operators that act on spaces of function on  $L^2(R^n)$  as follows

$$\hat{q}_k \psi(x) \equiv x_k \psi(x), \quad \hat{p}_k \equiv -i\hbar \frac{\partial \psi(x)}{\partial x_k} \quad k = 1 \dots n \quad (42)$$

Notice that the operator  $-i\hbar \frac{\partial \psi(x)}{\partial x_k}$  has as (generalized) eigenvectors the de Broglie's states of definite values of momentum. From this point of view the indeterminacy relations between position and momentum, justified by Heisenberg considering *virtual experiments*, is a consequence of the properties of the Fourier transform.

The similarity between the formulation of dynamics in Hamiltonian Mechanics and in Quantum Mechanics has its roots in the fact that the basic elements of the two formalisms have *the same algebraic structure*. If the hamiltonian in the classical case is taken to be  $H_{class}(q, p)$  the evolution of the observables is given by

$$\frac{dA_{class}}{dt} = \{A_{class}, H_{class}\} \quad (43)$$

where  $\{f, g\}$  is Poisson bracket.

Formally the solution of the Schrödinger equation  $i\hbar \frac{d\phi}{dt} = H\phi$  is  $\phi(t) = e^{-itH}\psi$ . By duality it follows that the evolution of the observables  $\hat{A}$  (operators in the Hilbert space in which the system is described) is described by the equation

$$\frac{d\hat{A}}{dt} = i[\hat{A}, H] \quad (44)$$

where  $[A_1, A_2] \equiv A_1 A_2 - A_2 A_1$  is the commutator of the matrices  $A_1, A_2$ .

The operation on the right hand side in (43) (which acts on functions on phase space) and that in (44) (which acts on bounded operators in a complex Hilbert space) have the same algebraic structure: they are  $*$ -derivations, i.e. the commute with taking adjoints, satisfy Leibnitz's rule and Jacobi's identity. Notice that in Quantum Mechanics the imaginary unit  $i$  takes the role of the symplectic structure  $J$  (recall that  $J$  is the imaginary unit in the presentation of the symplectic structure as complex structure). This algebraic homeomorphism was particularly emphasized by P. Dirac.

Soon after the formulation of Matrix Mechanics P. Dirac, who had become aware of those results without probably knowing many details, develops the *Quantum Algebra* [7]. In this very important paper Dirac introduces explicitly the terms *Quantum Algebra*, *Quantum Differentiation*, *Quantum Poisson Brackets* and remarks that the relation between Hamiltonian Mechanics and Quantum Mechanics lies in the isomorphism of the underlying algebraic structures.

Still, same care has to be taken in exploiting this relation because the algebra of functions on phase space is well defined while the algebra of unbounded operators in a Hilbert space must be treated with care. This leads to some difficulties if one attempts to formulate precisely the correspondence between the two theories.

## 6 Abstract Formulation

The formalism of Quantum Mechanics was later described in more mathematical terms by von Neumann [22], without restriction to the quantization of the canonical variables and connecting the formalism to the theory of algebras of operators in a (separable) Hilbert space. Very important contributions in this direction were made by A. Weyl; these Authors proved that, under suitable assumption, all representations of the canonical commutation relations are unitary equivalent. Later in these Lectures we will come back to this point and make more precise the statement of unitary equivalence.

Research on these more abstract aspects of Quantum Mechanics have led to major developments in the theory of  $C^*$ -algebras and of partial differential equations. It is safe to say that the main progress in these fields came through deepening the answers to questions that arise in Quantum Mechanics.

The exploitation of the structure of Quantum Mechanics and the need to refine the mathematical instruments led quickly to a distinction between researches on Quantum Mechanics: those with primary interest in the mathematical aspects and those with main interest in the properties of specific systems: atoms, molecules, crystals, semiconductors. The analysis of these systems have an independent mathematical interest and have greatly contributed to the field of Quantum Chemistry and Solid State Theory.

The first line of research has led to an axiomatic formulation of the theory and has laid the bases for the mathematical treatment of systems with infinitely many degrees of freedom (Quantum Field Theory, Algebraic Quantum Theory and Quantum Statistical Mechanics). This line of research favors in general algebraic structures.

The second line of research uses mostly Schrödinger's representation, and therefore its mathematics is mostly in the field of functional analysis and partial differential equations. This line of research benefits greatly from the *visualization* associated to the use of configuration space. The extraordinary success of Quantum Mechanics in the field of advanced technology comes from this line of research.

Both lines of research have put little emphasis on conceptual problems, e.g. on the *theory of measurement*, which is considered trivially solved in Classical Mechanics and is up to now far from being solved in Quantum Mechanics. We shall come back to this point in chapter “[Lecture 4: Entanglement, Decoherence, Bell's Inequalities, Alternative Theories](#)”.

## 7 Quantum Field Theory

Soon after the writing of Quantum Mechanics in quantum canonical variables, the structure was extended, at least formally, to system with an infinite number of degrees of freedom by Heisenberg and Pauli [11], Jordan and Pauli [15], and by Dirac [7].

The extension was naturally accomplished by choosing a basis of functions in the Hilbert space  $L^2(R^3)$  and promoting the functions in the basis chosen to be “quantum coordinates” satisfying Heisenberg commutation relations. A natural field of application is given by the Maxwell equations (quantum electrodynamics) and the Klein-Gordon equation (particle physics). Classically these systems are described by P.D.E. (partial differential equations) with a natural symplectic structure. The choice of a basis of functions  $f_k(t, x)$  turns this formalism into a system of differential equation in infinite dimension. These equations can be written, introducing a (formal) symplectic form, as Hamilton equations for an infinite set of harmonic oscillators.

One can *quantize* the system, at least formally, selecting a basis in  $L^2(R^3)$  and introducing quantum coordinates  $\hat{q}_k$ ,  $\hat{p}_k$  associated to the elements of the basis chosen. One can then define *quantum fields*  $\phi(t, x)$ ,  $\pi(t, x)$  by

$$\hat{q}_k \equiv \int \phi(t, x) f_k(x) d^3x, \quad \hat{p}_k \equiv \int \pi(t, x) f_k(x) d^3x \quad (45)$$

The basis can be chosen in such a way that the resulting commutation relations for the fields be (at least formally)

$$[\phi(t, x), \pi(t, y)] = i\delta(y - x) \quad [\phi(t, x), \phi(t, y)] = [\pi(t, x), \pi(t, y)] = 0 \quad x, y \in R^3 \quad (46)$$

where if  $z \in R^3$  one defines  $\delta(z) \equiv \delta(z_1)\delta(z_2)\delta(z_3)$ . The symbol  $\delta(w)$ ,  $w \in R^1$  (invented by Dirac) [7] is defined by

$$\int \delta(w - w') f(w') dw' = f(w) \quad (47)$$

for any continuous function  $f$ . In treating electrodynamics one has to pay special attention to gauge invariance. Notice that through (45)–(47) we have introduced *quantum fields* through which we describe the quantum mechanical version of the classical fields.

The formulation (46) through the use of Dirac distributions evidences *local properties* of the fields. It has set the basis for the treatment of the Quantized Electromagnetic Field and the development of Quantum Electrodynamics. An equivalent formulation has been given by Heisenberg and Pauli and later by Pauli and Wigner using proper bases in the Hilbert space. Although Jordan and Klein [12, 14] proved the equivalence of the two types of field quantization, Dirac's approach is remarkable for simplicity and clarity of exposition and has remained a milestone in Quantum Mechanics. It is reported in almost all textbooks on Quantum Field Theory and in almost all research papers. Only occasionally one finds reference to the more mathematically correct quantization which uses an orthonormal basis in the Hilbert space.

The fact that the system has now an infinite number of degrees of freedom gives rise to formal difficulties. These difficulties can be overcome in the case of a free field theory but if one introduces a *relativistic local* interaction between the fields one runs into very serious difficulties, mainly due to the distributional properties of the fields and to the need to control convergence of the formal series. The former can be attacked with appropriate redefinitions of products of distributions; convergence of the series is more difficult; in favorable cases one proves Borel summability.

Very soon Fock, and later Dirac, noticed that the *quantization of the fields* could be given a different form. Take for simplicity the case of the wave equation (massless Klein-Gordon equation) in one dimension

$$\frac{\partial^2}{\partial t^2} \phi(t, x) = \frac{\partial^2}{\partial x^2} \phi(t, x) \quad (48)$$

which in Fourier basis can be written

$$\frac{\partial^2}{\partial t^2} \hat{\phi}(t, k) = k^2 \hat{\phi}(t, k) \quad (49)$$

i.e. as an infinite (non-denumerable) collection of harmonic oscillators.

On the other hand, setting

$$a(k) = \frac{1}{\sqrt{2}}(\hat{p}(k) + i\hat{q}(k)), \quad a^* = \frac{1}{2}(\hat{p}(k) - i\hat{q}(k)) \quad (50)$$

it is easy to verify for each  $k$  that the operator  $a^*(k)a(k)$  is the hamiltonian of a quantum harmonic oscillator in  $L^2(R)$  with elastic constant  $|k|$ . This operator is selfadjoint and has (simple) eigenvalues  $(n + \frac{1}{2})k^2$ ,  $n = 0, 1, \dots$ ; the corresponding normalized eigenfunctions  $\psi_n(k)$  are the Hermite polynomials.

We have therefore obtained two representations of the scalar field of mass zero: one through the operators  $\hat{Q}(k)$ ,  $\hat{P}(k)$  and one through the operators  $a(k)$ ,  $a^*(k)$ .

The first is a quantization of the solutions of the wave equation. To each configuration of the classical field corresponds in this quantization a quantum state. This state can be written as superposition (with prescribed phases) of elements which an increasing number of particles (coherent states). This representation of the (quantized) free electromagnetic field which is commonly used in Quantum Optics.

The representation through the operators  $a_k$ ,  $a_k^*$  is particularly convenient when one introduces an interaction that does not preserve the number of particles. The quantization usually employed to describe the interaction of particles with the electromagnetic field (modulo difficulties connected with gauge invariance).

## 8 Anticommutation Relations

The Dirac-Fock representation is also interesting because it suggests how to provide in a simple way a Fock space for fermions through the introduction of anti-commutation relations. Indeed if  $f, g$  are test functions and  $a(f) \equiv \int a(x)f(x)dx$  we require that the following relations (anti-commutation relations) be satisfied

$$\{a(f), a^*(f)\} = |f|^2, \quad \{a(f), a(f)\} = a^2(f) = 0 \quad \{a^*(f), a^*(f)\} = (a^*(f))^2 = 0 \quad (51)$$

where  $\{b, c\} \equiv bc + cb$ . It follows that two fermions cannot be in the same state and  $n_f \equiv a^*(f)a(f)$  can be either zero or  $|f|^2 \cdot I$ .

This field quantization through *anticommutation relations* has the advantage of incorporation “Pauli statistics” (in an unpublished manuscript Jordan described what is now called Fermi-Dirac statistic and attributed it to Pauli) [1, 12, 13]. We shall discuss the anti-commutation relations in the second part of these Lecture Notes.

Jordan returned later to this field quantization in a paper together with Wigner [16] and gave an alternative derivation of the anti-commutation relations. Jordan arrived at the description of anti-commuting fields through an attempt to overcome the ambiguity in the order of operators in Quantum Mechanics. He defined a new product for operators that is symmetric the *Jordan product*. For two operators  $A, B$  it is defined as

$$A \cdot B \equiv \frac{1}{2}(AB + BA) \equiv \frac{1}{2}\{A, B\} \quad (52)$$



This product is commutative but not associative. It satisfies however a weak form of associativity

$$(A^2 \cdot B) \cdot A = A^2 \cdot (B \cdot A), \quad A^2 \equiv A \cdot A \quad (53)$$

Consider the bilinear operation on hermitian operators

$$[A, B] = \frac{i}{2}(AB - BA) \quad (54)$$

(the imaginary unit is there to assure hermiticity). This antisymmetric bilinear operation satisfies the Jacobi identity

$$[[A, B]C] + [[B, C]A] + [[C, A], B] = 0 \quad (55)$$

and therefore defines a Lie algebra structure. The lack of commutativity of the Jordan product is linked to this Lie structure by

$$(A \cdot B) \cdot C - A \cdot (B \cdot C) = [B, [A, C]] \quad (56)$$

and it is easy to see that bilinear forms in the operators  $a(f)$ ,  $a^*(f)$  satisfy (54)–(56) if and only if the anticommutation relations (51) are satisfied. Recalling the in classical electromagnetism the observable (currents, Poynting vector) are quadratic in the field this led naturally Jordan and Wigner to introduce fields that obey Fermi-Dirac statistics.

In this way Jordan in an unpublished manuscript arrived through his *Jordan algebra* to a formulation of what is now called *Fermi-Dirac statistics* for particles which satisfy Pauli's exclusion principle.

It should also be remarked that Jordan [13, 14] was the first to generalize the new Quantum Mechanics to a system with infinitely many degrees of freedom by *quantizing the wave function* and introducing a (formal) functional calculus for a collection of functions on  $\oplus_{n \in \mathbb{N}} L^2(\mathbb{R}^d)$ . This is a quantization adapted to the classical Lagrangian field formalism. One may say that the purpose of Jordan was to introduce as *configuration space* a space in which the points are substituted with suitable (generalized) functions. The quantized fields would appear as (non-commuting) functionals on this space. It was therefore more akin to the quantization of the solutions of the wave equation introduced later by I. Segal.

## 9 Algebraic Structures of Hamiltonian and Quantum Mechanics. Pauli's Analysis of the Spectrum of the Hydrogen Atom

We noticed that the basic structures with which time evolution is generated in both theories by derivations i.e. operations which are linear and satisfy Leibnitz's rule. In Hamiltonian Dynamics they are given by Poisson brackets on the algebra of

functions on phase space. In Quantum Dynamics they are given by fs on the algebra of observables. These structures satisfy Leibnitz' rule and Jacobi's identity and are algebraically isomorphic. This algebraic isomorphism allows to set up easily a perturbation theory in analogy with hamiltonian perturbation.

It was soon realized that in quantum mechanics perturbation theory does not have the difficulties which plagued the classical case and which were emphasized by H. Poincaré, namely the *small denominators problem*. This is due to the fact that in general no harmonics appear in the frequencies of an atom. Perturbation theory as developed by Born and Heisenberg in analogy with Hamiltonian dynamics is still at present at the basis of dynamics in quantum mechanics.

Pauli made use of this algebraic isomorphism to determine the energy spectrum of the hydrogen atom. As already mentioned this had a relevant role in the acceptance of Quantum Mechanics by the community of researchers in Physics.

The classical equation for the energy a particle with mass  $m$  attracted by a particle of mass  $M$  by the coulomb force is hamiltonian. The hamiltonian is in cartesian coordinates

$$H = \frac{p^2}{2\mu} - \frac{e}{r}, \quad r = |x| \quad (57)$$

where  $\mu$  is the reduced mass and  $e$  the charge.

The *stationary* Schrödinger equation for the Hydrogen atom is

$$\hat{H}\phi(x) = E\phi(x) \quad \hat{H} \equiv -\frac{\hbar^2 \Delta}{2\mu} - \frac{e}{|x|} \quad (58)$$

The quantum hamiltonian is derived from the classical one using the quantization we have described. In the analysis that follows we don't pay attention to domain problems (most of the operators considered are unbounded); a more refined analysis will be given in chapter "[Lecture 19: Estimates of the Number of Bound States. The Feshbach Method](#)".

Equation (58) had been solved by Schrödinger [21] providing the spectrum of the Hydrogen atom and the eigenfunctions. Following Pauli we use the correspondence between Poisson brackets and commutators to determine *the discrete part* of the spectrum of the operator (58).

In classical mechanics it is known the invariance of the Hamiltonian under spacial rotation implies that the angular momentum  $L \equiv q \wedge p$  is conserved. Correspondingly in quantum mechanics the momentum  $\hat{J} = \hat{x} \wedge \hat{p}$  is conserved (commutes with the Hamiltonian).

It is known in Hamiltonian mechanics that in the case of Coulomb (=Kepler) system there is a further vector which is constant of motion, the Runge-Lenz vector

$$R = \frac{p}{\mu} \wedge L - e^2 \frac{x}{|x|} \quad (59)$$

In hamiltonian mechanics the presence of this further integral of motion implies that the energy can be made to depend on only one action variable; the value of the two other constants of motion are determined by the parameters of the theory. This leads to a particularly simple solution of the equation of motion.

Pauli investigated the commutation relations of the hermitian part of the operator which is obtained from  $R$  applying the rules of the quantum correspondence. This hermitian part is

$$\hat{M} = (2\mu)^{-1} \hat{p} \wedge \hat{J} - (2\mu)^{-1} J \wedge \hat{p} - e^2 \frac{x}{|x|} \quad (60)$$

By using formally Heisenberg's commutation relations one can see that  $H$ ,  $M_k$ ,  $J_k$  satisfy (formally) the following commutation relations

$$\begin{aligned} [H, \hat{J}_k] &= 0, & [H, \hat{M}_k] &= 0 & [\hat{J}_i, \hat{J}_k] &= i\hbar\epsilon_{i,k,l}\hat{J}_l \\ [\hat{J}_m, \hat{M}_k] &= i\hbar\epsilon_{i,k,l}\hat{M}_l & [\hat{M}_j, \hat{M}_k] &= \frac{2\hbar}{i\mu}\epsilon_{j,k,l}\hat{J}_l H \end{aligned} \quad (61)$$

$$\hat{J} \cdot \hat{M} = \hat{M} \cdot \hat{J} = 0, \quad (\hat{M})^2 - e^2 = \frac{2}{\mu} \hat{H}(\hat{J})^2 + \hbar^2 \quad (62)$$

Since  $\hat{J}$  and  $\hat{M}$  commute with the hamiltonian it is possible to restrict oneself to a representation in which the hamiltonian is diagonal and negative (bound states).

Consider a subspace in which the Hamiltonian has value  $E < 0$ . Introducing the operator  $\tilde{M}_i = \frac{\mu}{2|E|}^{\frac{1}{2}} \hat{M}_i$  one verifies that the vector valued operators  $\frac{\hat{J} \pm \tilde{M}}{2}$  commute and the components of each pair satisfy the commutation relations of angular momentum. Hence

$$(\hat{J} + \tilde{M})^2 = 4\hbar^2 j_1(j_1 + 1) \quad (\hat{J} - \tilde{M})^2 = 4\hbar^2 j_2(j_2 + 1) \quad (63)$$

where  $j_1, j_2$  may take integer or half-integer values. But  $\hat{J} \cdot \tilde{M} = \tilde{M} \cdot \hat{J} = 0$  and therefore

$$(\hat{J} + \tilde{M})^2 = (\hat{J} - \tilde{M})^2 \quad (64)$$

and  $j_1 = j_2 \equiv j$ .

Assume for the moment that  $2j$  can take any integer value. We derive from (62)

$$\frac{2e}{\mu}(\tilde{M}^2 + \hat{J})^2 + m\hbar^2 = m - e^2 \quad (65)$$

and then

$$(\tilde{M}^2 + \hat{J}^2 n + \hbar^2)4[(\tilde{M} + \hat{J})^2 + (\tilde{M} - \hat{J})^2] + \hbar^2 = \hbar^2(2j + 1)^2$$

It follows

$$E = -\frac{\mu e^2}{2\hbar^2} \frac{1}{(2j+1)^2} \quad (66)$$

The procedure we have followed shows also that the degeneracy of the levels is  $(2j+1)^2$ .

The commutation relations (61) and (62) are those of the generators (properly normalized) of the Lie algebra  $so(4)$ . Since  $SO(4)$  is semisimple and the representation of  $so(4)$  is irreducible the representation lifts to an irreducible representation of  $SO(4)$ .

This analysis can be done also in the Schrödinger representation but is more cumbersome (the operator  $\tilde{M}$  is in the Schrödinger representation a second-order differential operator).

The work of Pauli, based on the newly established homeomorphism between commutators and Poisson brackets had a relevant role in the acceptance of the new Mechanics by the community of theoretical physicists.

## 10 Dirac's Theorem

For the description of dynamics the formulation given by Schrödinger and by Heisenberg depend heavily on analogies with hamiltonian dynamics. The systematic use made by von Neumann of a Hilbert space structure and of the structure of the algebra of operators acting on this space makes no longer necessary for the description of dynamics to choose in advance a representation (a special presentation of the Hilbert space). We shall see in chapter “[Lecture 5: Automorphisms; Quantum Dynamics; Theorems of Wigner, Kadison, Segal; Continuity and Generators](#)” that the structure of Quantum Mechanics as described by its axioms has in itself a natural definition of evolution (of dynamics), *independent of classical analogies*. Of course specific problems, that have a classical analogue, benefit from analogies with the hamiltonian formalism of classical dynamics. And then the best choice of representation is determined by the specific problem at hand.

While quantum dynamics can be obtained without reference to the isomorphism between commutators and Poisson brackets, the structural rigidity of the connection of dynamics in Quantum Mechanics with the hamiltonian structure Classical Dynamics is well described by the following theorem due to Dirac.

Recall that in Hamiltonian Dynamics the vector field on the space of differentiable function on phase space that describes the evolution under the action of a hamiltonian  $H$  is a *derivation* (satisfies Leibnitz' rule and the Jacobi identity).

An analogous structure exists for matrices. Let  $M_n$  be the algebra of rank  $n$  matrices; a linear operator  $\delta$  on  $M_n$  is called a *derivation* if it satisfies Leibnitz's rule for the product. It is a *star-derivation* if  $\delta(a^*) = (\delta(a))^*$  for  $a \in M_n$ , where  $a^*$  is the Hermitian conjugate of  $a$ . We shall say that the derivation  $\delta$  is an *inner derivation* if there exists  $h \in M_n$  such that  $\delta(a) = i[h, a]$ .

**Theorem** (Dirac) *Every  $*$ -derivation of  $M_n$  is inner (and the matrix  $h$  can be chosen to be hermitian).*

We shall give in the course of these Lectures a proof of Dirac's theorem placing it in the more general setting of operator theory on infinite dimensional Hilbert spaces and  $C^*$ -algebras (Bratteli). We remark here that Dirac's theorem implies that every linear dynamics on  $M_n$  has the form

$$i \frac{da}{dt} = ha - ah \quad (67)$$

where the matrix  $h$  is hermitian and unique modulo addition of a term proportional to the identity  $I \in M_n$ . The solution of (67) is  $a(t) = e^{-ith} a e^{ith}$ . One can interpret Dirac's theorem by saying that (in finite dimensions) every quantum vector field is hamiltonian and every evolution is unitary.

## References

1. Baccigaluppi, G., & Valentini, V. (2009). *Quantum theory at the crossroad*. Cambridge: Cambridge University Press.
2. Born, M. (1924). *Zeitschrift für Physik*, 26, 379–395.
3. Bohr, N., Kramers, H., & Slater, J. (1924). *Philosophical Magazine*, 47, 785–802.
4. Born, M., & Jordan, P. (1952). *Zeitschrift für Physik*, 34, 858–888.
5. Born, M., Jordan, P., & Heisenberg, W. (1926). *Zeitschrift für Physik*, 35, 557–581.
6. Dirac, P. A. M. (1926). *Proceedings of the Royal Society A*, 112, 661–676.
7. Dirac, P. A. M. (1927). *Proceedings of the Royal Society A*, 114, 243–265.
8. The Principles of Quantum Mechanics Oxford University Press 198.
9. Eckart, P. (1926). *Physics Review*, 28, 711–726.
10. Heisenberg, W. (1925). *Zeitschrift für Physik*, 33, 879–893.
11. Heisenberg, W., & Pauli, W. (1927). *Annalen der Physik*, 81, 109–139.
12. Jordan, P. (1925). *Zeitschrift für Physik*, 30, 297–319.
13. Jordan, P. (1927). *Zeitschrift für Physik*, 45, 765–783.
14. Jordan, P. & Klein, O. (1927). *Zeitschrift für Physik*, 75–94.
15. Jordan, P., & Pauli, W. (1928). *Zur Quantenelektrodynamik ladungsfreie Felder Zeits. für Physik*, 47, 151–173.
16. Jordan, P., & Wigner, P. (1928). *Über das Paulische Äquivalenzverbot. Zeitschrift für Physik*, 47, 631–655.
17. Kramers, (1924). *Nature*. 113, 673–676.
18. Lademburg, R. (1921). *Zeitschrift für Physik*, 4, 451–468.
19. Pauli, W. (1926). *Letter to Jordan*.
20. Pauli, W. (1926). *Zeitschrift für Physik*, 36, 336–363.
21. Schrödinger (1926). *Annalen der Physik*, 81, 109–139.
22. von Neumann, J. (1927). *Nachrichten von der Gesellschaft der Wissenschaften zu Göttingen*, 1–57.
23. van Velt. (1924). *Physics Review*, 24, 330–365.

Lectures on the Mathematics of Quantum Mechanics I

DellAntonio, G.

2015, XXI, 459 p., Hardcover

ISBN: 978-94-6239-117-8

A product of Atlantis Press