Complex Coordinates and Quantum Mechanics

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By introducing complex canonical coordinates, classical and quantum mechanics may be embedded in the same formulation. In such a way, the connection between Poisson brackets and commutators, canonical transformations and unitary transformations, etc., become apparent. This formulation is also particularly suitable for discussing the classical limit of quantum mechanics and for quantum-statistical mechanics.

I. INTRODUCTION

The general structures of classical and quantum mechanics are usually regarded as essentially different and the relation between them has been the subject of several investigations.[1] As a matter of fact, the connection between the usual formulation of classical mechanics and quantum mechanics is not immediate. The classical limit of quantum mechanics, which is usually identified with the limit $\hbar \rightarrow 0$, is rather obscure; the connection between commutators and Poisson brackets is difficult to explain in that limit. Neither is the connection between the theory of canonical transformations and unitary transformations in quantum mechanics apparent, and one has to rely on analogy arguments.

A better understanding of the relation between the two theories may be obtained by a formal theory of generalized dynamics which includes classical and quantum mechanics as special cases. This is realized by a more general formulation of Hamiltonian mechanics, with the introduction of complex canonical variables. Hamilton's equations, Poisson brackets, and canonical transformations exhibit an elegant and compact form, when written in terms of the new variables. In particular the analysis of canonical transformations reduces to the study of the analytical properties of the generating functions as functions of the new variables.

Quantum mechanics may be regarded as a special case of the above formulation. The Schrödinger equation may in fact be written as Hamilton equations for complex canonical coordinates, the Hamiltonian function being the mean value of the Hamiltonian operator. In this formulation the analogy between classical and quantum mechanics goes beyond the formal structure of the equations of motion. In the same way as for the Hamiltonian, a "classical" phase function of complex variables may be introduced for any other observable and for them the Poisson brackets may be defined as in the classical case. Thus, the quantum problem takes a form similar to that of a classical problem; for example the Poisson bracket of two conjugate variables has the same value 1 in both the classical and quantum cases.

Most of the assumptions of quantum mechanics have a natural explanation in the framework of complex classical mechanics, in which they have a strictly related analog. For example, the correspondence between Poisson brackets and commutators is not arbitrary: the Poisson bracket of two "classical" phase functions is in fact the mean value of the commutator between the corresponding operators. Similarly, the hermiticity of observables has its analogue in the fact that the phase functions of complex variables must satisfy a reality condition, and the unitarity condition is nothing but the canonicity condition for generating functions in the case of complex canonical coordinates.

Thus, classical and quantum mechanics may be embedded in the same formulation, the "classical" form of quantum mechanics being obtained by taking the mean values of the corresponding operators. The difference between the two theories does not lie in their mathematical structures, but rather in the way a physical problem is schematized and reduced to a mathematical problem. For example, the system of one single particle is completely described by *six* variables in classical mechanics, whereas an *infinite* number of canonical variables is needed in quantum mechanics. In particular, as we show below, a quantum particle is equivalent to a set of infinite classical harmonic oscillators. This aspect of the theory is emphasized by second quantization or field theory. As a matter of fact, both classical and quantum mechanics have the structure of a Lie group of transformations associated with a Lie algebra of functions of the canonical variables. The two formulations may be regarded as different representations of the same algebraic structure, the difference being in the number of dimensions of the space in which the representation is realized.

Thus, the classical limit of quantum mechanics may be understood as an approximation in which the dynamical variables are described by average values: $q_{\text{class}} = \langle \Psi \mid q \mid \Psi \rangle$, $p_{\text{class}} = \langle \Psi \mid p \mid \Psi \rangle$ etc., in which the "hidden" quantum structure of the state is neglected.

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[1] J. Von Neumann, Ann. Math. **33**, 587, (1932); U. Uhlhorn, Arch. Phys. **11**, 87 (1956); H. J. Groenewold, Physica **12**, 405 (1946); E. Wigner, Phys. Rev. **40**, 749 (1932); T. F. Jordan and E. C. Sudarshan, Rev. Mod. Phys. **33**, 515 (1961); etc.

The limit $\hbar \to 0$ should be better understood as a condition on the magnitude of the dynamical variables involved in a specific problem in order that the above approximation is valid (Ehrenfest theorem).

II. COMPLEX VARIABLES AND CLASSICAL MECHANICS

The state of a classical system is completely described by the real canonical coordinates q_k, p_k, $k=1, \cdots, N$ (N being the number of degrees of freedom) and the time evolution is governed by the Hamilton equations

$$\dot{q}_k = \partial H/\partial p_k, \qquad \dot{p}_k = -\partial H/\partial q_k. \tag{1}$$

In the place of the variables q_k, p_k, which play a nonsymmetric role in Eqs. (1), we introduce the variables z_k and $z_k{}^*$ so defined[2]

$$z_k = (q_k + ip_k)/\sqrt{2}, \qquad z_k{}^* = (q_k - ip_k)/\sqrt{2}.$$

In terms of the new variables, the Hamilton equations take the compact form:

$$i\dot{z}_k = \partial H/\partial z_k{}^*, \qquad -i\dot{z}_k{}^* = \partial H/\partial z_k. \tag{2}$$

The second set of equations may be obtained from the first by complex conjugation, and it is therefore superfluous. In Eqs. (2), the Hamiltonian has to be regarded as a function of z_k and $z_k{}^*$, satisfying the reality condition:

$$H(z, z^*) = [H(z, z^*)]^* \equiv H^*(z^*, z). \tag{3}$$

Like the Hamiltonian, any other phase function $f(q, p)$, may be written in terms of the variables z, z^* and the analogue of Eq. (3) is satisfied by definition:

$$f(z, z^*) = [f(z, z^*)]^*. \tag{3'}$$

For any two phase functions $f(z, z^*)$ and $g(z, z^*)$, the Poisson bracket is given by:

$$\{f, g\} \equiv \frac{\partial f}{\partial q_k}\frac{\partial g}{\partial p_k} - \frac{\partial f}{\partial p_k}\frac{\partial g}{\partial q_k} = -i\left(\frac{\partial f}{\partial z_k}\frac{\partial g}{\partial z_k{}^*} - \frac{\partial f}{\partial z_k{}^*}\frac{\partial g}{\partial z_k}\right)$$
$$\equiv -i[f, g]. \tag{4}$$

The sum over repeated indices is implied. The bracket [,], defined before may be regarded as a definition of the Poisson bracket in the new variables. As is evident from Eqs. (2) and (4), the variables z_k and $z_k{}^*$ play the role of canonical *conjugate* variables, just as the old q's and p's.

[2] By a suitable choice of the system of units or by a simple similarity transformation, the variables q and p may be made to have the same dimensions.

III. CANONICAL TRANSFORMATIONS

We are now in the position of characterizing the canonical transformations in terms of the new variables. They are implicitly defined by the property of leaving the Poisson brackets invariant. However, as far as the study of canonical transformations is concerned, it is useful to give a differential characterization.

In the usual formulation, a transformation from the variables q, p to the variables Q, P is canonical if the following condition is satisfied:

$$p_k\dot{q}_k - P_k\dot{Q}_k - H + K = dF/dt,$$

where $H=H(q, p)$ and $K=K(Q, P)$ are the Hamiltonians in the two systems of coordinates and F is an arbitrary function. When the complex variables are used, the above equation is equivalent to:

$$K(Z, Z^*) - H(z, z^*) + \tfrac{1}{2}i[Z_k\dot{Z}_k{}^* - \dot{Z}_kZ_k{}^* - z_k\dot{z}_k{}^* + z_k{}^*\dot{z}_k] = dF/dt.$$

The above condition may be transformed into a set of differential equations. For this purpose, a system of independent variables has to be chosen, with the prescription that part of them belong to the old system and part to the new one. In the usual formulation, one may choose either p, Q or P, q or p, P or q, Q. Now one may choose either z, Z or z^*, Z^* or z, Z^* or z^*, Z. Then one has, e.g., in the first case:

$$K(z, Z) - H(z, Z) + \tfrac{1}{2}i[Z_k\dot{Z}_k{}^* + \dot{Z}_kZ_k{}^* - 2\dot{Z}_kZ_k{}^* - (z_k\dot{z}_k{}^* + \dot{z}_kz_k{}^*) + 2\dot{z}_kz_k{}^*] = dF/dt$$

or

$$K - H + i[\dot{z}_kz_k{}^* - \dot{Z}_kZ_k{}^*] = \frac{\partial F^{(1)}}{\partial z_k}\dot{z}_k + \frac{\partial F^{(1)}}{\partial Z_k}\dot{Z}_k + \frac{\partial F^{(1)}}{\partial t}.$$

The above condition is equivalent to the set of differential equations:

$$iz_k{}^* = \partial F^{(1)}/\partial z_k, \quad -iZ_k{}^* = \partial F^{(1)}/\partial Z_k, \quad K - H = \partial F^{(1)}/\partial t. \tag{5}$$

Similarly, one has, in the other cases,

$$-iz_k = \partial F^{(2)}/\partial z_k{}^*, \qquad iZ_k = \partial F^{(2)}/\partial Z_k{}^*, \tag{6}$$

$$iz_k{}^* = \partial F^{(3)}/\partial z_k, \qquad iZ_k = \partial F^{(3)}/\partial Z_k{}^*, \tag{7}$$

and

$$-iz_k=\partial F^{(4)}/\partial z_k^*, \qquad -iZ_k^*=\partial F^{(4)}/\partial Z_k. \qquad (8)$$

Here, $F^{(1)}=F^{(1)}(z, Z)$, $F^{(2)}=F^{(2)}(z^*, Z^*)$, $F^{(3)}=F^{(3)}(z, Z^*)$, and $F^{(4)}=F^{(4)}(z^*, Z)$ may be regarded as the generating functions of the transformations. It is not difficult to see that there are only two independent sets of generating functions. Equations (6) and (8) may in fact be obtained by (5) and (7) by complex conjugation. Therefore,

$$F^{(2)}(z^*, Z^*)=[F^{(1)}(z, Z)]^*,$$

$$F^{(4)}(z^*, Z)=[F^{(3)}(z, Z^*)]^*.$$

Thus, of the four types of generating functions of the usual theory, only two are really different, in each pair the two functions being the real and imaginary part of the same analytic function. Apart from a greater elegance and simplicity, the reduction from four to two is in agreement with what one would expect from a group theoretical point of view. The two types of generating functions classify, in fact, the transformations which are connected with the identity and those which are not.

The integrability conditions for Eqs. (7) and (8) are:

$$\frac{\partial^2 F}{\partial z_i \partial Z_k^*}\frac{\partial^2 F^*}{\partial z_i^* \partial Z_l}+\frac{\partial^2 F}{\partial Z_k^* \partial Z_i^*}\frac{\partial^2 F^*}{\partial Z_i \partial Z_l}=\delta_{kl},$$

$$\frac{\partial^2 F}{\partial z_i \partial z_k}\frac{\partial^2 F^*}{\partial z_i^* \partial z_l^*}+\frac{\partial^2 F}{\partial z_k \partial Z_i^*}\frac{\partial^2 F^*}{\partial z_l^* \partial Z_i}=\delta_{kl}, \qquad (9)$$

Hence, defining

$$F_{ik}=F_{ki}\equiv\partial^2 F/\partial Z_i^*\partial Z_k^*, \qquad F_{ki}^\dagger\equiv F_{ik}^*,$$

$$f_{ik}=f_{ki}\equiv\partial^2 F/\partial z_i\partial z_k, \qquad f_{ki}^\dagger\equiv f_{ik}^*,$$

$$g_{ik}\equiv\partial^2 F/\partial z_i\partial Z_k^*, \qquad (g^\dagger)_{ki}\equiv g_{ik}^*,$$

Eqs. (9) and (10) take the form of matrix equations

$$g^\dagger g+F^\dagger F=I, \qquad (10)$$

$$gg^\dagger+ff^\dagger=I. \qquad (11)$$

Here I denotes the unit matrix. The set of Eqs. (7), (10), and (11) define a canonical transformation connected with the identity.

Similarly, from Eqs. (5) and (6) one has

$$\frac{\partial^2 F'}{\partial z_i \partial z_k}\frac{\partial^2 F'^*}{\partial z_i^* \partial z_l^*}-\frac{\partial^2 F'}{\partial z_k \partial Z_i}\frac{\partial^2 F'^*}{\partial z_l^* \partial Z_i^*}=\delta_{kl},$$

$$\frac{\partial^2 F'}{\partial Z_i \partial Z_k}\frac{\partial^2 F'^*}{\partial Z_i^* \partial Z_l^*}-\frac{\partial^2 F'}{\partial z_i \partial Z_k}\frac{\partial^2 F'^*}{\partial Z_l^* \partial z_i^*}=\delta_{kl},$$

or, with obvious notations,

$$f'f'^\dagger-hh^\dagger=I, \qquad (12)$$

$$F'^\dagger F-h^\dagger h=I. \qquad (13)$$

In this formulation, canonical transformations may be studied by investigating the analytic properties of the generating functions. For example, conformal transformations of phase space, i.e., transformations which preserve the angles, are characterized by analytic functions[3]

$$Z_k=Z_k(z), \qquad Z_k^*=Z_k^*(z^*).$$

On the other hand, the conditions (10), (11) require

$$g^\dagger g=gg^\dagger=I,$$

F_{ik} and f_{ik} vanishing in this case. Thus, one has

$$Z_k=a_{ki}z_i, \qquad Z_k^*=a_{ki}^*z_i^*,$$

$$a_{ik}a_{il}^*=a_{ik}^*a_{il}=\delta_{kl},$$

i.e., the only canonical transformations preserving the angles in phase space are the linear orthogonal transformations. In a similar way, the transformations that preserve angles except for their sign, are the inverse conformal transformations. By conditions (12), (13) they are restricted to linear "orthogonal" transformations with determinant -1:

$$Z_k=Z_k(z^*)=a_{ki}z_i^*, \qquad Z_k^*=Z_k^*(z)=a_{ki}^*z_i,$$

$$a_{ki}a_{li}^*=a_{ik}a_{il}^*=-\delta_{kl}.$$

We list now some cases of canonical transformations that take a simple expression in the above formulations. We restrict ourselves to rotations in the planes q_k, p_k:

$$Z_k=z^{i\alpha}kz_k, \qquad Z_k^*=\exp(-i\alpha_k)z_k^*,$$

The above transformation is equivalent to the following transformation of the real canonical coordinates:

$$Q_k=(\cos\alpha_k)q_k-(\sin\alpha_k)p_k,$$

$$P_k=(\sin\alpha_k)q_k+(\cos\alpha_k)p_k,$$

Thus for $\alpha_k=\frac{1}{2}\pi$, the exchange of p and q is obtained,

$$Q_k=-p_k, \qquad P_k=q_k,$$

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[3] H. Cartan, *Théorie élémentaire des fonctions analytiques d'une ou plusieurs variables complexes* (Hermann & Cie., Paris, 1961).

whereas for $\alpha_k=\pi$, the space inversion is obtained,

$$Q_k=-q_k, \qquad P_k=-p_k.$$

(Note that it is continuously connected with the identity.) The generating function is

$$F=-i\exp(-i\alpha_k)z_k^*Z_k.$$

therefore if the Hamiltonian is invariant under the above transformation, the quantity

$$2z_k^*Z_k\exp(-i\alpha_k)=2z_kz_k^*=q_k^2+p_k^2$$

is a constant of motion. This means that the modulus of the two-dimensional vector $(q_k,\ p_k)$ is conserved. This is the case of the harmonic oscillator, when the variables

$$q_k=(m\omega_k)^{\frac{1}{2}}x_k, \qquad p_k=m\dot{x}_k/(m\omega_k)^{\frac{1}{2}}$$

are chosen as canonical variables. (The transformation from $q_k'=x_k$, $p_k'=m\dot{x}_k$ to q_k, p_k is obviously a canonical transformation.)

IV. "CLASSICAL" FORM OF QUANTUM MECHANICS

An interesting application of the above formulation is given by quantum mechanics.[4] To this purpose we consider a system of particles, contained in a box of finite volume Ω. The Hilbert space $\mathcal{H}$ of the states of the system has infinite but numerable dimensions. For example, one may take as basic states the eigenstates of the momentum, spin, etc. of each particle; because of the finite volume Ω, the eigenvalues of the components of the momentum of each particle are discrete and numerable. For simplicity sake, we further assume that the energy spectrum is bounded, i.e., the energy of the system cannot exceed a definite, arbitrary large value $\bar{E}$. Then, we may restrict ourselves to a subspace $\mathcal{H}'\subseteq\mathcal{H}$ of finite dimensions. The above assumptions are not restrictive since one may make $\Omega\rightarrow\infty$ and $\bar{E}\rightarrow\infty$ at the end of calculations, then making $\mathcal{H}'$ go to $\mathcal{H}$.

The generic state $|\Psi\rangle$ may be written as a superposition of the basic states $|\alpha_k\rangle$, $k=1,\cdots,N$, which form a complete orthonormal set

$$|\Psi\rangle=u_k\,|\alpha_k\rangle$$

(sum over k is implied), where u_k are complex coefficients which completely determine the state $|\Psi\rangle$, once the basic states $|\alpha_k\rangle$ are fixed. As we see below, the coefficients u_k may be regarded as a sort of canonical coordinates and the complex $2N$-dimensional euclidean space of the u_k's may be regarded as the phase space of our quantum system.[4]

On using the Schrödinger picture for the state vectors, and taking the basic states as time-independent, the Schrödinger equation may be written as $(\hbar=c=1)$

$$i(d\,|\Psi\rangle/dt)=i(du_i/dt)\,|\alpha_i\rangle=H\,|\alpha_i\rangle u_i$$

or

$$i(du_k/dt)=\partial\mathcal{H}/\partial u_k^*=\langle\alpha_k\,|\,H\,|\,\alpha_i\rangle u_i,$$

where

$$\mathcal{H}\equiv H_{ki}u_k^*u_i\equiv\langle\alpha_k\,|\,H\,|\,\alpha_i\rangle u_iu_k^*=\langle\Psi\,|\,H\,|\,\Psi\rangle.$$

In that form the Schrödinger equation is nothing but the Hamilton equations in complex canonical coordinates for a classical system whose Hamiltonian function is the mean value of the quantum Hamiltonian operator. We shall call $\mathcal{H}$ the "classical" Hamiltonian.

Introducing the real coordinates

$$q_k\equiv(1/\sqrt{2})(u_k+u_k^*), \qquad p_k\equiv(i/\sqrt{2})(u_k^*-u_k),$$

the "classical" Hamiltonian becomes

$$\mathcal{H}=\tfrac{1}{2}H_{ki}(q_iq_k+p_ip_k+iq_kp_i-iq_ip_k).$$

This is the Hamiltonian for N coupled harmonic oscillators. An interesting case is when the Hamiltonian is one of the basic observables. Then

$$H_{ki}=E_k\delta_{ki}$$

(because of a possible degeneracy not all the E_k are different, i.e., it may be $E_k=E_l$ even if $k\neq l$). In this case, one has

$$\mathcal{H}=\tfrac{1}{2}E_k(q_k^2+p_k^2).$$

This is equivalent to using *normal* canonical coordinates for describing a system of classical harmonic oscillators.

The above-shown analogy between quantum and classical mechanics goes beyond a formal structure of the equations of motion. All the physical quantities may be expressed as bilinear functions of the variables u_k, u_k^*:

$$\langle\Psi\,|\,B\,|\,\Psi\rangle=\langle k\,|\,B\,|\,i\rangle u_k^*u_i\equiv b_{ki}u_k^*u_i\equiv\mathcal{B}(u,u^*).$$

The hermiticity condition for observables requires

$$b_{ki}=\langle k\,|\,B\,|\,i\rangle=\langle i\,|\,B^\dagger\,|\,k\rangle^*=\langle i\,|\,B\,|\,k\rangle^*=b_{ik}^*.$$

[4] This formulation is particularly suitable in quantum statistical mechanics, see: F. Strocchi, "An Axiomatic Approach to Statistical Mechanics" (to be published).

Therefore,

$$\mathcal{B}(u, u^*) = [\mathcal{B}(u, u^*)]^*;$$

this is just condition (3′). Thus, with any observable, one may associate a real phase function of the complex variables u, u^*.

One of the basic quantities in classical mechanics is the Poisson bracket. Then, given any two Hermitian operators A and B, we may define the Poisson bracket between the corresponding phase functions $\mathcal{A}$ and $\mathcal{B}$, as in classical mechanics:

$$[\mathcal{A}, \mathcal{B}] \equiv \frac{\partial\mathcal{A}}{\partial u_k}\frac{\partial\mathcal{B}}{\partial u_k^*} - \frac{\partial\mathcal{A}}{\partial u_k^*}\frac{\partial\mathcal{B}}{\partial u_k}$$

$$= a_{ik}u_i^* b_{kl}u_l - a_{ki}u_i b_{lk}u_l^*$$

$$= \langle i \mid AB - BA \mid l \rangle u_i^* u_l = \langle [A, B] \rangle,$$

i.e., the classical Poisson bracket $[\mathcal{A}, \mathcal{B}]$ between the quantities $\mathcal{A}$ and $\mathcal{B}$ is the mean value of the commutator $[A, B]$ between the corresponding operators. Thus, the "classical" form of quantum mechanics leads necessarily to the usual correspondence between classical Poisson brackets and quantum commutators.

V. CANONICAL OR UNITARY TRANSFORMATION IN QUANTUM MECHANICS

A transformation of the Hilbert space into itself may be regarded as generated by a linear operator U, thus yielding

$$U \mid \Psi \rangle = u_k' \mid \alpha_k \rangle = U_{ki}u_i \mid \alpha_k \rangle,$$

where

$$U_{ki} \equiv \langle k \mid U \mid i \rangle \equiv \langle i \mid U^\dagger \mid k \rangle^*.$$

Hence, on defining

$$U_{ki}^\dagger = \langle k \mid U^\dagger \mid i \rangle,$$

one has

$$U_{ki} = (U_{ik}^\dagger)^*.$$

If the operator U has an inverse U^{-1}, one gets

$$u_k = (U^{-1})_{ki}u_i', \qquad U_{ki}^{-1} \equiv \langle k \mid U^{-1} \mid i \rangle.$$

The above transformation of the Hilbert space is therefore equivalent to a transformation of the complex canonical variables according to:

$$u_k' = U_{ki}u_i.$$

On requiring that the above transformation is canonical, one obtains as generating functions

$$F = iU_{ki}u_k'^* u_i,$$

and conditions (10) and (11) imply

$$U_{ki}U_{li}^* = U_{ik}U_{il}^* = \delta_{kl},$$

i.e.,

$$U^\dagger U = UU^\dagger = I.$$

Thus, unitary transformation in quantum mechanics are canonical transformations in the sense of classical mechanics.

From the generating function F, it is easy to see that

$$U_{ki}u_k'^* u_i = u_k^* u_k = u_k'^* u_k'$$

is a constant of motion, i.e., the norm of state vectors is conserved.

It is interesting to note that a large class of canonical transformations, corresponding to the classical transformations of Eqs. (5), (6), (12), and (13) have not been considered in quantum mechanics. For them, one has:

$$U^\dagger U = UU^\dagger = -I,$$

i.e., they change the sign of the metric in Hilbert space. However, from a physical point of view, an Hilbert space with negative definite metric is acceptable just as one with positive definite metric. Then, one should expect that transformations of kind (1), (2) should be used in quantum mechanics, e.g., for representing discontinuous transformations such as, e.g., charge conjugation etc.