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Quantization Postulate in Quantum Mechanics

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Abstract

The procedure of transition from classical observables to quantum (operator) observables in quantum mechanics is discussed. By an example it is shown that, even in simple cases, the method of self-adjoint extensions of formal differential expressions for defining physical observables as operators is not equivalent to the procedure of forming operator functions corresponding to these observables. This inequivalence is not a formal one but has physical consequences connected with the compatibility of observables.

As is well known (see von Neumann, 1932), every observable of a quantum mechanical system is usually represented by a self-adjoint operator in the Hilbert space H of states of the system. Since some of the observables [e.g., the energy $E(p_1, p_2, p_3)$] can be functions of other observables (e.g., momentum components p_1, p_2, p_3), the definition of operator $E(p_1, p_2, p_3)$ in H may be regarded as forming an operator function of the operators p_1, p_2, p_3 given in H. Such a procedure of giving operator sense to certain expressions (of defining them as operators) is usually called the quantization postulate, or correspondence principle in quantum mechanics. (As is known, some of the quantum systems may be regarded as counterparts—via the correspondence principle—of classical systems described by quantities and relations similar to those in the quantum case.) Sometimes it is convenient to consider the set of quantum mechanical observables as particular operator representations in a suitable Hilbert space of some abstract quantities obeying certain commutation relations (such as, for instance, the case of coordinate and momentum). The choice of a particular Hilbert space corresponds to a particular realization of the quantum system.

In cases when functions of non-commuting operators are formed, their definition can be ambiguous owing to the order in which the non-commuting operators enter as factors in some products. [A discussion of this point is given, for example, by von Neumann (1932) and by other authors. Our discussion below does not concern this type of ununiqueness.]

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On the other hand, from the Schrödinger equation (for instance, of a free particle with mass m) it is evident that energy E (or square of momentum $\mathbf{p}^2$) can be regarded on a suitable class of differentiable functions as the operator

$$E = -\hbar^2/2m \sum_{i=1}^{3} \partial^2/\partial x_i^2$$

and

$$\mathbf{p}^2 = -\hbar^2 \sum_{i=1}^{3} \partial^2/\partial x_i^2$$

Then the operator corresponding to the quantum mechanical observable of energy (or square of momentum) could be considered in some cases also as a self-adjoint extension of E (or $\mathbf{p}^2$), defined on some dense domain in H. A similar method of extending formal symmetric differential expressions is frequently used in practical applications of quantum mechanics as another procedure of defining observables mathematically (see, for example, Wightmann, 1964, Part II, §8; Kato, 1966, Chap. 5, §5).

In the sequel, assuming the validity of some natural physical conditions, the inequivalence of the above two procedures is discussed. The application of one of them to a quantum mechanical example leads to compatible (commuting) observables while the other procedure defines incompatible (non-commuting) observables.

A single quantum particle is considered, whose energy $E(\mathbf{p}, m_i^*)$ as a function of momentum $\mathbf{p} = \{p_1, p_2, p_3\}$ has the form[1]

$$E(\mathbf{p}, m_i^*) = \sum_{i=1}^{3} p_i^2/2m_i^*, \qquad m_1^* \neq m_2^* \neq m_3^*, m_i^* > 0, i = 1, 2, 3 \tag{1}$$

and the square of momentum $\mathbf{p}^2$ is given by

$$\mathbf{p}^2 = p_1^2 + p_2^2 + p_3^2 \tag{2}$$

The particle is moving in a bounded three-dimensional domain D (considered as an open set in the three-dimensional Euclidean space) which is a potential well with infinitely high walls. (The wave functions are zero on the boundary σ of D.) Domain D is different from a parallelepiped with faces parallel to coordinate planes, and the boundary σ is smooth. A physical realization of the above quantum mechanical situation can be the motion of a quasiparticle (an exciton, or a magnon, or an electron) in the periodic field of a non-isotropic crystal piece of the form D. The interaction with such a non-isotropic periodic field is described by introducing new "effective" masses m_i^* of the particle (see Kittel, 1960). The motion is such that the quasiparticle is prevented from sticking to the surface of D. (The quasiparticle with effective masses m_i^* can evidently exist only inside D.) This discussion is valid for values of $\mathbf{p}$ small enough and a crystal piece D large enough that the "dispersion law" $E(\mathbf{p}, m_i^*)$ can be approximated ("effective mass approximation") by quadratic function

[1] The quantities m_i^*, $i = 1, 2, 3$ are considered as constants.

(1) of "quasimomentum" **p** (see Kittel, 1960). In the sequel, equality (1) is postulated as an exact law. Consequently, in this approximation, the motion of the quantum particle can be described equivalently by the "quantization" of the motion of a classical particle with the Hamiltonian (1).

According to von Neumann (1932), the Hilbert space of states of the above quantum system can be realized as the set of all square integrable functions $L_2(D)$ defined on D. Let us denote by S_1 (or, respectively, S_2) the formal differential expressions

$$S_1 = \sum_{i=1}^{3} \frac{1}{2m_i^*} \frac{\partial^2}{\partial x_i^2} \tag{3}$$

$$S_2 = \sum_{i=1}^{3} \frac{\partial^2}{\partial x_i^2} \tag{4}$$

As discussed above, $-\hbar^2 S_1$ (or, respectively, $-\hbar^2 S_2$) can correspond to the energy (or, respectively, square of momentum) of the quasiparticle if they are defined on suitable domains and then extended to linear self-adjoint operators in the Hilbert space H. Let us denote by S_1', S_2' the operators defined by (3) and (4), respectively, on the common domain $C^\infty(\bar{D})$ consisting of all functions infinitely differentiable on $\bar{D}$, vanishing on the boundary σ of D, and continuous together with all their derivatives on $\bar{D}$ (the closure of $\bar{D}$). As any ψ $[\psi \in C^\infty(\bar{D})]$ vanishes on σ, so ψ may be (*a priori*) a physically interesting state of our quantum system. Thus, from physical considerations we assume that self-adjoint operators S_1^N and S_2^N corresponding to the energy and square of momentum of the quasiparticle should be self-adjoint extensions of the (symmetric) operators S_1' and S_2', respectively [i.e., domains of definition of S_1^N, S_2^N should contain $C^\infty(\bar{D})$]. The existence and uniqueness of such extensions is ensured by the following mathematical facts. For the operators S_1', S_2' it is known (see Dunford and Schwartz,1963, Chap. XIV, 6, Theorem 25), that the closures $\bar{S}_1'$ and $\bar{S}_2'$ of S_1' and S_2', respectively, are self-adjoint operators. Then, clearly, $\bar{S}_1'$ (or, respectively, $\bar{S}_2'$) is the unique self-adjoint extension of S_1' (or, respectively, S_2') because $\bar{S}_1'$ ($\bar{S}_2'$) is by definition the smallest closed extension of S_1' (S_2') and at the same time its largest closed extension in virtue of the maximality of any self-adjoint operator. The above-stated uniqueness gives the only possibility of defining von Neumann's observables S_j^N by equalities $S_j^N \equiv \bar{S}_j'$, $j = 1, 2$. Let us denote by S_1^0 and S_2^0 the operators defined by (3) and (4), respectively, on a common domain $C_0^\infty(D)$ consisting of all infinitely differentiable in D functions with compact supports, contained in D.

According to the general theorem proved by Denchev (1970) and applied to the present particular case, the Friedrich's self-adjoint extensions S_1^F and S_2^F of the operators S_1^0 and S_2^0, respectively, do not commute[2] for the special choice of domain D. Furthermore, it is known (see Denchev, 1970 beginning

[2] Two self-adjoint operators are said to commute, if their spectral resolutions commute, (see also von Neumann, 1932). According to Denchev's theorem, S_1^F and S_2^F commute if and only if D is a parallelepiped with faces parallel to coordinate planes.

of proof of Theorem I), that S_1^F (S_2^F) is an extension of S_1' (S_2'), i.e.,

$$S_1^F \supset S_1', \qquad S_2^F \supset S_2' \tag{5}$$

Since any self-adjoint operator is closed, and $\bar{S}_j'$ is the smallest closed extension of S_j', clearly

$$S_j^F \supset \bar{S}_j' \supset S_j', \qquad j = 1, 2 \tag{6}$$

Using the proved uniqueness of $\bar{S}_j'$ as a self-adjoint extension of S_j' (6) becomes: $S_j^F = \bar{S}_j' \supset S_j'$. As a result (using the definition $S_j^N \equiv \bar{S}_j'$, $j = 1, 2$), self-adjoint operators S_1^N and S_2^N corresponding to the energy and square of momentum do not commute, if one defines these operators by the procedure of self-adjoint extensions [and assume—from physical considerations—that their domains of definition contain $C^\infty(\bar{D})$].

One can follow another procedure of giving operator sense to the relations (1) and (2) as discussed above. Let H be the Hilbert space of states corresponding to the physical system in consideration. For instance, $H = L_2(D)$ or some other arbitrary realization of H. Suppose, three commuting self-adjoint operators p_1, p_2, p_3 are defined in H so that they are admissible as candidates for three components of the momentum of the quasiparticle. It is known (see Plesner, 1965, Theorem 9.4.7) that p_1, p_2, p_3 can be regarded as operator functions of one and the same self-adjoint operator. If operator functions (1) and (2) are formed, (see Dunford and Schwartz, 1963, Chap. XII. 2, 8 Corollary), operators $E(\mathbf{p}, m_i^*)$ and $\mathbf{p}^2$ commute in any particular realization of H as functions of the same self-adjoint operator.

Remark. In the particular realization $H = L_2(D)$ operator functions $E(\mathbf{p}, m_i^*)$ and $\mathbf{p}^2$ cannot, for instance, be defined on the set of functions $C^\infty(\bar{D})$ by differential expressions (3) and (4). If this were the case, then $E(\mathbf{p}, m_i^*)$ and $\mathbf{p}^2$ would be commuting self-adjoint extensions of S_1' and S_2', respectively, contrary to the above-proved non-commutativity of S_j^N, $j = 1, 2$—the unique self-adjoint extensions of S_j', $j = 1, 2$.

So the two considered procedures of quantization of (1) and (2) are in general not equivalent. In quantum mechanics (see von Neumann, 1932), commutativity of two observables is equivalent to their compatibility. This has nontrivial physical consequences, e.g., occurrence (or absence) of uncertainty relations.

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