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Critical View on the Heisenberg-Robertson Uncertainty Relation

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Mathematical properties of the Heisenberg and Robertson uncertainty relations, the basis of entire quantum theory, are reviewed. The ordinary proof of the Heisenberg uncertainty relation for coordinate and corresponding momentum is based on the Cauchy-Schwarz inequality. Transition to uncertainty relation for mean square deviation from this inequality requires to confine operators by some fundamental restrictions, such as hermiticity, equal domains, self-adjointness etc. After the needed restrictions are applied, it follows inequality, which is a source of uncertainty relations for various operators. D.Judge and K.Kraus well before mentioned that the commutation relation for two operators do not imply fulfilment of uncertainty relation automatically, but it is necessary to impose some strong mathematical restrictions. In explicit calculation appearing of surface terms is expected, which can introduce a non-zero contribution into the uncertainty relation. Below we give an algorithm for explicit calculation of these surface contributions. We study the relation between an angle and momentum operator, which was the subject of current investigation in the last years.

Uncertainty relation, commutators, orbital momentum and angle

The uncertainty relation forms the basis of entire quantum theory. The ordinary proof of the Heisenberg uncertainty relation for coordinate and corresponding momentum is based on the Cauchy-Schwarz inequality, which is a general property of Hilbert space. For a pair of operators A and B, acting on the state $|\psi\rangle$, the Schwartz inequality gives

$$\langle A\Psi | A\Psi\rangle \langle B\Psi | B\Psi\rangle \geq \left|\langle A\Psi | B\Psi\rangle\right|^2 \tag{1}$$

Transition to the uncertainty relation for *variance (or mean square deviation)* $\left|\langle \Delta A \Delta B\rangle\right|$, where $\Delta A \equiv A - \langle A\rangle$, requires to impose some limitations on operators under consideration, such as Hermiticity, unique domains, self-adjointness etc. After that such limitations are fulfilled, the general uncertainty relation for any such operators reduces to

$$\left|\langle \Delta A \Delta B\rangle\right|^2 \geq \frac{1}{4}\left|\langle [A, B]\rangle\right|^2, \tag{2}$$

which is a source of uncertainty inequalities (Here $\hbar = 1$ unites is used).

However, it was pointed out earlier [1,2], that the commutation relation

$$\left[\hat{A},\hat{B}\right] = i\hat{C} \tag{3}$$

for quantum mechanical observables $\hat{A},\hat{B}$ and $\hat{C}$ by itself does not imply the uncertainty relation

$$\langle \Delta A \Delta B \rangle \geq \frac{1}{2}\left|\langle C \rangle\right| \tag{4}$$

for all physically interesting states. There are examples showing that the uncertainty relation (2) for any two observables $\hat{A}$ and $\hat{B}$ is not valid in such a generality. For example, the uncertainty relation for $\hat{A}$ and $\hat{B}$ is usually written in the form (2)

$$\Delta_\psi A \Delta_\psi B \geq \frac{1}{2}\left|(\psi, i\left[\hat{A},\hat{B}\right]\psi)\right|, \tag{5}$$

where $\left(\Delta_\psi A\right)^2 = \left\|\left(\hat{A} - \langle \hat{A}_\psi \rangle 1\right)\psi\right\|^2$, with $\langle \hat{A}_\psi \rangle = \left(\psi, \hat{A}\psi\right)$ and likewise for $\hat{B}$. This definition is used in many papers [3-5]. Thus the left-hand side of relation (5) is defined for $\psi \in D(A) \cap D(B)$. On the other hand, the right-side is only defined on the subspace $D([A,B]) = D(AB) \cap D(BA)$, which is much smaller in general.

However, A and B being self-adjoint, relation (1.5) can be rewritten in the form [2,3]

$$\Delta_\psi A \Delta_\psi B \geq \frac{1}{2}\left|i\left(A\psi, B\psi\right) - i\left(B\psi, A\psi\right)\right|, \tag{6}$$

where the domain of the right-hand side now coincides with that of the left-hand side, $D(A) \cap D(B)$, i.e. the product of uncertainties for two observables A and B is not determined by their commutator, but by the Hermitian sesquilinear form [2]

$$\Phi_{A,B}\left(f,g\right) = i\left(Af, Bg\right) - i\left(Bf, Ag\right), \quad \text{for all } f,g \in D(A) \cap D(B). \tag{7}$$

As it is mentioned in [3], this modification is not simply a cosmetic one. When A or B are operators of differentiation, the surface terms occurring upon integration by parts do not vanish in general and contribute to the uncertainty relations.

Specific situation occurs in 3-dimensions, when spherical coordinates are used. One of the basically coordinates, namely, a distance, is restricted by a half-line. Therefore, we have to be careful in calculation of surface integrals, which, because of boundary conditions at the origin, may also give the nontrivial contributions.

While the strong mathematical consideration is most powerful [3], the explicit calculation has more transparency and simplicity. It was already demonstrated clearly in number of papers [6,7], concerning the Ehrenfest theorem. We are inclined to think that a similar simplification may also occurr in case of uncertainty relations.

General Consideration of the Heisenberg-Robertson Relation

We derive the uncertainty relation following to a Weil method [8]. Suppose that the commutation relation between two Hermitian operators has the form (3), where C is an Hermitian operator too.Consider the integral

$$J(\alpha)=\int\left|(\alpha A_1-iB_1)\psi\right|^2 d\tau\geq 0, \tag{8}$$

where $A_1=A-a,\ B_1=B-b$ with α,a,b are some real parameters. Now

$$J=\int\left((\alpha A_1-iB_1)\psi\right)^*(\alpha A_1-iB_1)\psi d\tau=\int(\alpha A_1+iB_1)\psi^*(\alpha A_1-iB_1)\psi d\tau. \tag{9}$$

Despite the fact that A and B are Hermitian operators, we write down the Hermiticity condition with some care. Introducing the following notations

$$\int(A_1\psi)^* A_1\psi d\tau=\int\psi^* A_1^2\psi d\tau+Q_1 \tag{10}$$

$$\int(B_1\psi)^* B_1\psi d\tau=\int\psi^* B_1^2\psi d\tau+Q_2 \tag{11}$$

$$\int(A_1\psi)^* B_1\psi d\tau=\int\psi^* A_1B_1\psi d\tau+X \tag{12}$$

$$\int(B_1\psi)^* A_1\psi d\tau=\int\psi^* B_1A_1\psi d\tau+Y \tag{13}$$

Here Q_1,Q_2,X,Y are surface terms, remaining after integration by parts, which maybe non-vanishing on the boundaries. They show deviations from (6). Exactly these terms can modify the uncertainty relations.

Let us drown an analogy between above decomposition and that given in paper [5]. The *expectation commutator* was introduced in the following way

$$A\neq B:=\langle A\psi\,|\,B\psi\rangle-\langle\psi\,|\,AB\psi\rangle \tag{14}$$

and instead of (5), new uncertainty relation was considered

$$\Delta A\Delta B\geq\frac{1}{2}\left|A\neq B-B\neq A+\langle[A,B]\rangle\right|. \tag{15}$$

The extra term here corresponds to ours $X-Y$. Therefore, our consideration is equivalent to that of [5].Taking into account notations above, the sought-for integral (8) can be rewritten in the following form (assumed the normalization of the state ψ)

$$J=\int\psi^*\left(\alpha^2A_1^2-i\alpha[A_1,B_1]+B_1^2+Q_1+Q_2+i\alpha(Y-X)\right)\psi d\tau=$$

$$=\alpha^2\langle A_1^2\rangle-i\alpha\langle[A_1,B_1]\rangle+\langle B_1^2\rangle+Q_1+Q_2+i\alpha(Y-X) \tag{16}$$

and after taking into account the commutation relations $[A_1,B_1]=[A,B]=iC$, we find

$$\alpha^2\langle A_1^2\rangle+\alpha\langle C+i(Y-X)\rangle+\langle B_1^2\rangle+Q_1+Q_2\geq 0. \tag{17}$$

Now from positive definiteness of square trinomial, we conclude that

$$\langle A_1^2\rangle\left[\langle B_1^2\rangle+Q_1+Q_2\right]\geq\frac{1}{4}\langle C+i(Y-X)\rangle^2. \tag{18}$$

If we now return to above introduced notations and suppose in addition that $a=\langle A\rangle$ and $b=\langle B\rangle$, it follows generalized Heisenberg relation

$$\left\langle (\Delta A)^2\right\rangle\left\langle\left[(\Delta B)^2+Q_1+Q_2\right]\right\rangle\geq\frac{1}{4}\left\langle C+i(Y-X)\right\rangle^2, \tag{19}$$

where $(\Delta A)^2=(A-\langle A\rangle)^2$ and the uncertainty inequality takes the final form

$$\left\langle(\Delta A)\right\rangle\sqrt{\left\langle(\Delta B)^2\right\rangle+Q_1+Q_2}\geq\frac{1}{2}\left|\left\langle C+i(Y-X)\right\rangle\right|. \tag{20}$$

Some comments are now in order here:

This relation reduces to the usual one (2), when $Q_1=Q_2=X=Y=0$, i.e. when all considered operators are *self-adjoint*. For physical operators a more strict conditions are needed: it is necessary that not only wave function ψ, but also $B\psi$ belongs to the appropriate domain, where A is Hermitian (and similarly, $A\psi$ must remain in the domain of wavefunctions, where B is Hermitian). In general, uncertainty product $\langle(\Delta A)\rangle\langle(\Delta B)\rangle$ does not always separated as a factor. As a rule, it appears in combination with Q_1 or Q_2. In this respect the Weil method, as such, is inconvenient to use. But the same happens in using other known methods, which are described in various textbooks [9,10]. As we will see below, explicit calculation gives that the additional terms from Eq. (10) – (13) *does not always disappear.* Only in cases, when additional terms are absent, it follows the Heisenberg- Robertson (4) uncertainty relation.

When operators commute, $C=0$ and, therefore, the two physical quantities are measured simultaneously, i.e. one, obviously, can take $\langle(\Delta A)\rangle=\langle(\Delta B)\rangle=0$. Then it follows from (19) a true inequality, $0\geq-\frac{1}{4}\langle(Y-X)\rangle^2$. Hence (19) also contains a case of simultaneous measurement of two physical quantities.

It may happen that not all surface terms are zero simultaneously. As we will see below it depends on the singular character of considered operators at the boundaries.

If $Q_1+Q_2<0$, then $(\Delta B)^2$ is constrained from below, $\left\langle(\Delta B)^2\right\rangle>|Q_1+Q_2|$. In contrast, when $Q_1+Q_2>0$, then $(\Delta A)^2$ is constraint

$$(\Delta A)\geq\frac{1}{2}\left|\left\langle C+i(Y-X)\right\rangle\right|\frac{1}{\sqrt{Q_1+Q_2}}. \tag{21}$$

So, one can establish which physical quantity will be constraint from below. In the following we get examples of application of (20). As usual, minimization of uncertainty relation corresponds to the sign of equality in (20).

Uncertainty Relation between Orbital Momentum and Angle

The most papers are devoted to the momentum-angle uncertainty relation [1,2,4]. We begin our consideration from this example. Let us choose in (19) the following operators

$$A=L_Z=-i\hbar\frac{d}{d\varphi},\qquad B=f(\varphi), \tag{22}$$

where $f(\varphi)$ is a real function, not involving differentials with respect to φ. The domain of the azimuthal angle is restricted to the interval $[0,2\pi]$, and since the wave functions $\psi(\varphi)$ are continuously differentiable, they must fulfill the boundary conditions [5]

$$\psi(0)=\psi(2\pi); \qquad \left.\frac{d\psi(\varphi)}{d\varphi}\right|_{\varphi=0}=\left.\frac{d\psi(\varphi)}{d\varphi}\right|_{\varphi=2\pi}. \tag{23}$$

In this case [Eq.(10)]

$$\int_0^{2\pi}(L_Z\psi)^* L_Z\psi\, d\varphi=\int_0^{2\pi}\psi^* L_Z^2\psi\, d\varphi+\hbar^2\left(\psi(\varphi)\frac{d\psi^*}{d\varphi}\right)_0^{2\pi} \tag{24}$$

and, so

$$Q_1=\hbar^2\left(\psi(\varphi)\frac{d\psi^*}{d\varphi}\right)_0^{2\pi}=\hbar^2\left\{\psi(2\pi)\left(\frac{d\psi^*}{d\varphi}\right)_{2\pi}-\psi(0)\left(\frac{d\psi^*}{d\varphi}\right)_0\right\}. \tag{25}$$

Because of boundary conditions (23), the last term vanishes and so $Q_1=0$. Moreover, $Q_2=0$, as $f(\varphi)$ is a multiplication operator. Then, in case of (23) we derive

$$\int_0^{2\pi}(L_Z\psi)^* f(\varphi)\psi\, d\varphi=\int_0^{2\pi}\psi^* L_Z f(\varphi)\psi(\varphi)\, d\varphi+i\hbar(f(\varphi)|\psi(\varphi)|^2)_0^{2\pi}. \tag{26}$$

Therefore,

$$X=i\hbar(f(\varphi)|\psi(\varphi)|^2)_0^{2\pi}=i\hbar|\psi(0)|^2[f(2\pi)-f(0)]. \tag{27}$$

In addition, (13) reads

$$\int_0^{2\pi}(f(\varphi)\psi)^* L_Z\psi\, d\varphi=\int_0^{2\pi}\psi^* f(\varphi)L_Z\psi\, d\varphi. \tag{28}$$

Hence, $Y=0$. Taking into account all of these relations in (20), one concludes that

$$\left\langle(\Delta L_Z)^2\right\rangle\left\langle(\Delta f(\varphi))^2\right\rangle\geq\frac{\hbar^2}{4}\left\langle-\frac{df}{d\varphi}+|\psi(0)|^2(f(2\pi)-f(0))\right\rangle^2. \tag{29}$$

Note that analogous relation was derived in [5]. In case,when $f(\varphi)=\varphi$, it follows

$$\left\langle(\Delta L_Z)^2\right\rangle\left\langle(\Delta\varphi)^2\right\rangle\geq\frac{\hbar^2}{4}\left(1-2\pi|\psi(0)|^2\right). \tag{30}$$

If $\psi(\varphi)$ functions are not periodic functions, then instead of (29) one has

$$\left\langle(\Delta L_Z)\right\rangle\sqrt{(\Delta f(\varphi))^2+Q_1}\geq\frac{\hbar}{2}\left|\left\langle-\frac{df}{d\varphi}+\left\{|\psi(2\pi)|^2 f(2\pi)-|\psi(0)|^2 f(0)\right\}\right\rangle\right|. \tag{31}$$

The same results were found in papers [3,4,5]. We see that the inclusion of extra terms modifies Robertson's uncertainty relation, following from the "ordinary" commutation relation $[\varphi,L_Z]=i\hbar$. The reason is well known: The orbital momentum operator given by Eq.(22) is Hermitian only in the space of periodic functions with period 2π, but $\varphi\psi(\varphi)$ is not in domain, where L_Z is a self-adjoint operator. If one choses the function $f(\varphi)$ to be periodic also, then the extra terms vanish as well.

ფიზიკა

ჰაიზენბერგ-რობერტსონის განუზღვრელობათა თანაფარდობის კრიტიკული შეფასება

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ნაშრომში ახლებური თვალსაზრისით განიხილება ჰაიზენბერგისა და რობერტსონის განუზღვრელობათა თანაფარდობის მათემატიკური ასპექტები, რაც წარმოადგენს კვანტური მექანიკის საფუძველს. კოორდინატასა და შესაბამის იმპულსს შორის თანაფარდობის ჩვეულებრივი მტკიცება ემყარება კოშისა და შვარცის უტოლობას. ამ უტოლობიდან განუზღვრელობათა თანაფარდობაზე გადასვლა ოპერატორის საშუალო კვადრატული გადახრისათვის მოითხოვს ოპერატორებზე ფუნდამენტური შეზღუდვების დადებას, როგორიცაა, ერმიტულობა, განსაზღვრის არეები, თვითშეუღლებულობა და ა.შ. ამ შეზღუდვების გამოყენების შემდეგ მიიღება უტოლობა, რომელიც წარმოადგენს განუზღვრელობათა თანაფარდობის წყაროს სხვადასხვა ოპერატორისათვის. დ. ჯაჯის და კ. კრაუსის მიერ შენიშნული იყო, რომ კომუტაციის თანაფარდობა ჯერ კიდევ არ ნიშნავს განუზღვრელობათა თანაფარდობის თავისთავად შესრულებას, არამედ აუცილებელია გარკვეული მათემატიკური სიმკაცრის შეზღუდვები. როგორც ირკვევა, გამოთვლისას შესაძლებელია წარმოიშვას არანულოვანი ზედაპირული წევრები, რომლებიც წვლილს შეიტანენ თანაფარდობის საბოლოო სახეში. მიღებულია ამ ზედაპირული წევრების გამოთვლის ახალი ალგორითმი, რომელიც იძლევა მათი ანალიზის საშუალებას. შესწავლილი გვაქვს კუთხესა და იმპულსის მომენტის ოპერატორს შორის თანაფარდობა, რომელსაც ემღვნებოდა არსებულ ნაშრომთა უმრავლესობა. ცხადი გამოთვლებით ადვილად მიიღება შესწორებული თანაფარდობა.

REFERENCES

1. Judge D. (1964) On the uncertainty relation for angle variables.*Nuovo Cim*., **31**:332.
2. Kraus K. (1967) A further remark on uncertainty relations, *Zeitschrift fur physic*., **201**: 134.
3. Gieres F. (2000) Mathematical surprises and Dirac's formalism in quantum mechanics., *Rep.Prog. Phys*., **63**: 1893.
4. Chisolm E.(2001) Generalizing the Heisenberg uncertainty relation., *Am.J.Phys.,* **69**:368.
5. Renziehausen K. and Barth I. (2019) How to generalize the Ehrenfest theorem and the uncertainty principle. ArXiv:quant-ph1904.06177.
6. Khelashvili A. and Nadareishvili T. (2020) Hypervirial and Ehrenfest theorems in spherical coordinates: systematic approach. *Phys. Particles and Fields*., **51**:107.
7. Khelashvili A. and Nadareishvili T. (2021) Application of modified Hypervirial and Ehrenfest theorems and several their consequences. *Phys. Particles and Fields*., **52**: 155.
8. Davidov A.S. (2011) Kvantovaia mekhanika, BXV Peterburg (in Russian).
9. Shankar R. (2008) Principles of quantum mechanics, 2nd edition. Plenum Press. N.Y.
10. Greiner W. (2008) Quantum mechanics. Springer. Berlin.

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