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Physics

Possible Incompatibility between the Heisenberg-Robertson Uncertainty Relation and the Principles of Quantum Mechanics

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According to the Heisenberg uncertainty principle the product of uncertainties for measurement of noncommuting the observables in quantum theory are restricted from below by the mean value of commutator of corresponding operators in any state. In almost all textbooks of quantum mechanics the source of this relation is the general form, derived by Robertson. It should be marked that in spite of its great relevance, the Heisenberg-Robertson relation was criticized in scientific papers. The results are found which contradict to this relation. The aim of this paper to find new cases when the above mentioned relation fails as well. It is shown that the average value of commutator of non-commuting Hermitian operators appearing in the Heisenberg-Robertson uncertainty relation may be zero for some wave functions. Explicit examples of Coulomb, modified Coulomb and singular oscillator are considered and demonstrated that the right-hand-sides of commutators become zero, when they are averaged by corresponding wave functions.

uncertainty relation, commutator, non-commuting operators, variance, standard deviations, inequality

There is almost common belief based on the textbooks treatment of the (uncertainty) problem that if one has a pair of non-commuting observables A and B, then the product of standard deviations ΔA and ΔB calculated for them is always larger than some nonzero positive number, say c:

$$\Delta_\psi A \cdot \Delta_\psi B \geq \frac{1}{2}\left|\left\langle \psi \left| i\left[A,B\right]\psi\right\rangle\right| \geq c > 0 . \tag{1}$$

In fact, $c \sim \hbar$ (Plank's constant). Here $\Delta_\psi A = \left\|\left(A - \left\langle A\right\rangle_\psi I\right)\psi\right\|$, with $\left\langle A\right\rangle_\psi = \left\langle \psi, A\psi\right\rangle$ and likewise for B. Inequality (1) is known as Heisenberg-Robertson (HR) uncertainty relation [1, 2]. It is remarkable to note that such a belief may lead to confusions. Thus, for example, analyzing general uncertainty relations, K.Urbanowski [3,4] has shown that there can exist such pairs of non-commuting observables A and B and such vectors that the lower bound for the product of standard deviations ΔA and ΔB, calculated for these vectors is zero: $\Delta A \cdot \Delta B \geq 0$. He suggested that it is not necessary for A and B to commute, $\left[A,B\right]=0$, in order that $\left\langle\left\langle \psi\left[A,B\right]\right|\psi\right\rangle = 0$ for some $\left|\psi\right\rangle \in \mathcal{H}$. Simply it may happen that for some $\left|\psi\right\rangle \in \mathcal{H}$ and for some non-commuting operators A and B the expectation value of the commutator $[A,B]$ vanishes $\langle\langle\psi[A,B]|\psi\rangle=0$. As A and B are observables, they are Hermitian or self-adjoint operators. It is easy to convince that the zero result may happen in cases, when ψ is an eigenvector of either A or B . Consider one example, illustrated this. The fundamental uncertainty relation has the form $[x,p_x]=i\hbar$, from which by using the Schwartz inequality, it follows the Heisenberg uncertainty principle

$$\Delta x\cdot\Delta p\geq\frac{\hbar}{2}. \tag{2}$$

Let ψ_p be a normalized eigenfunction of momentum operator $\hat{p}$. Owing to Hermiticity we derive

$$(\psi_p,[\hat{x},\hat{p}]\psi_p)=(\psi_p,\hat{x}\hat{p}\psi_p)-(\psi_p,\hat{p}\hat{x}\psi_p)=p\left[(\psi_p,\hat{x}\psi_p)-(\psi_p,\hat{x}\psi_p)\right]=0. \tag{3}$$

If, on the other hand, we first calculate the commutator, it follows

$$(\psi_p,[\hat{x},\hat{p}]\psi_p)=i\hbar(\psi_p,\psi_p)=i\hbar\neq 0. \tag{4}$$

The solution of this obvious paradox is difference in mathematical properties of momentum operator for different regions (domains), according to which this operator is a self-adjoint one or not in considered domain or does not belong to domain of $\hat{p}\hat{x}$. The knowledge about operator domain is critical and could not be ignored in practical calculations. Moreover, in semi-finite or finite intervals canonical commutation relation and uncertainty relation contradict to each other's. Real problem is that we are dealing with unbounded operators, such as momentum operator, which is a unbounded differential operator. Another example follows directly from the fundamental commutator

$$\left[x^2,\hat{p}_x\right]=i2\hbar x. \tag{5}$$

Taking its average by arbitrary vector ψ , one derives on the right-hand side the expression

$$\int_{-\infty}^{\infty}x|\psi(x)|^2\,dx. \tag{6}$$

It could be zero for any symmetric interval, because under integrand we have an odd function. Similarly, one can find many analogous results.The motivation of this paper is to examine such and similar cases and discuss other limitations of Robertson-Schrodinger uncertainty relation (1) .

Last period there appear many generalizations of Heisenberg-Robertson inequality (see [5]). These generalizations are directed to apply stronger mathematical apparatus and amplification of mathematical properties of operators under consideration. While the case of matrices are simple algebraic examples, more interesting from quantum mechanical point of view is an example of quantum particle in a box, spatial motion of which is restricted to a finite (confined) volume [4], namely in the segment $[a,b]$. It is an example of one-dimensional motion in a potential with boundaries. Therefore, the boundary conditions become essential. For example, in total real line the position operator and the momentum operator both are self-adjoint operators, but the problem is that in a segment considered, with vanishing conditions at the endpoints of this segment, there is no a self-adjoint operator acting as $-i\hbar\frac{d}{dx}$ in the subspace of square integrable functions in $L^2([a,b])$ [6]. Therefore, the change of boundary conditions (or the domain of this operator) is necessary for perform a self-adjoint extension of the momentum operator. It is worthwhile to note that in 3-dimensions and spherical coordinates the radial distance is defined only in a half-line, $0\leq r<\infty$. Therefore, formally we have deal with confined area and with one dimensional problem, but closer to realistic physics. Hence it is interesting to see, how the consideration in a restricted area exhibits the above-mentioned consequences (phenomena).

Below we consider more realistic models in three dimensions.

Calculation of Commutators

Our anxiety will be the relation between pair $A = r^2$ and $B = p^2$. Both of them are Hermitian operators. For calculation of their commutator, we make use an obvious relation

$$p^2 = p_r^2 + \frac{\hat{L}^2}{r^2}, \tag{7}$$

where $\hat{L}^2$ is a square of orbital momentum operator and p_r is a Hermitian radial component of linear momentum operator

$$p_r = -i\hbar\left(\frac{d}{dr} + \frac{1}{r}\right), \tag{8}$$

which obeys the following canonical commutation relation $\left[r, p_r\right] = i\hbar$. Now taking into account that r^2 is a 3-dimensional scalar and commutes with the angular momentum operator, we deduce

$$\left[r^2, p^2\right] = \left[r^2, p_r^2\right]. \tag{9}$$

The following steps are straightforward and one can obtain

$$\left[r^2, p^2\right] = 4\hbar^2\left(r\frac{\partial}{\partial r} + \frac{3}{2}\right). \tag{10}$$

Therefore, we must calculate the following average

$$\Delta r^2 \cdot \Delta p^2 \geq \left|\left\langle\left[r^2, p^2\right]\right\rangle\right|^2 = 4\hbar^2\left\langle r\frac{\partial}{\partial r} + \frac{3}{2}\right\rangle. \tag{11}$$

Let us calculate r.-h.-side of Eq. (11) for the attractive Coulomb potential, which has a form

$$V = -\frac{e^2}{r}. \tag{12}$$

The wave function is [7]

$$R_{nl} = C_{nl} r^l e^{-\frac{Br}{2n}} F\left(-n_r, 2l+2; \frac{Br}{n}\right) \; ; \; n = n_r + l + 1, \tag{13}$$

where

$$C_{nl} = \frac{B^{3/2}}{\sqrt{2n^2}\,(2l+1)!}\sqrt{\frac{(n+1)!}{n_r!}}\left(\frac{B}{n}\right)^l \tag{14}$$

is a normalization constant and

$$B = \frac{2me^2}{\hbar^2} = \frac{2}{a_0}; \qquad a_0 = \frac{\hbar^2}{me^2} \text{ - Bohr's radius.} \tag{15}$$

Our aim now is a calculation of average value $\left\langle r\frac{d}{dr}\right\rangle$. Derivative of hypergeometric function F, which occurs in this calculation, can be replaced by the known relation [8]

$$F'(a,b;x) = \frac{a}{b}F(a+1, b+1; x), \tag{16}$$

and then appearing integrals transform according to the Suslov's relation for reducing of hypergeometric function in terms of the Laguerre polynomials [9]

$$F\left(-n,\beta+1;x\right)=\frac{n!\Gamma\left(\beta+1\right)}{\Gamma\left(\beta+1+n\right)}L_n^{\beta}\left(x\right). \quad (17)$$

After straightforward calculations we derive the final result

$$\left\langle r\frac{d}{dr}+\frac{3}{2}\right\rangle=\frac{3}{2}+\frac{1}{2n}\left\{-3\left(l+1\right)+n_r\left[\frac{2\left(l+1\right)\left(4l+9-3n_r\right)}{2l+2+n_r}-3n_r-4l-6\right]\right\};\ n=n_r+l+1. \quad (18)$$

You can evidently see that for $n_r=0$ and arbitrary l, this expression vanishes! Operators under consideration r^2 and p^2 are non-commuting, moreover their commutator is a nontrivial operator again. And its average is zero in a modeless state.

Other Potentials

The same happens for several other realistic potentials such as: valence electron model, singular oscillator etc., For details of solutions see [10]. The further straightforward calculation and

repeating all procedures, exploited above, gives the following results, correspondingly:

- For the *v*alence electron model (or modified Coulomb) potential

$$V=-\frac{\alpha}{r}-\frac{V_0}{r^2}, \quad (19)$$

It follows

$$\left\langle r\frac{d}{dr}+\frac{3}{2}\right\rangle=\left|\frac{3}{2}+\frac{1}{\left(2n_r+2P+1\right)}\left\{-\frac{3}{2}\left(2P+1\right)+n_r\left[\frac{\left(2P+1\right)\left[2\left(2P+2\right)+3\left(1-n_r\right)\right]}{1+2P+n_r}-4P-3n_r-4\right]\right\}\right|, \quad (20)$$

where

$$P=\sqrt{\left(l+1/2\right)^2-2mV_0/\hbar^2}. \quad (21)$$

As in previous case, here at $n_r=0$ and for arbitrary l the expression (20) vanishes again.

- For the singular oscillator potential

$$V=-\frac{V_0}{r^2}+gr^2; \qquad \left(V_0>0,\ \ g>0\right) \quad (22)$$

it follows [10]

$$\left\langle r\frac{d}{dr}+\frac{3}{2}\right\rangle=2n\frac{P+n}{P+n+1}; \qquad n=0,1,2,..., \quad (23)$$

where P is given by (27) again. Here also for $n=0$ and arbitrary l we derive vanishing result.

For pure oscillator potential ($V_0=0$) it follows:

$$\left\langle r\frac{d}{dr}+\frac{3}{2}\right\rangle=2n\frac{2l+2n+1}{2l+2n+3}; \qquad n=0,1,2,... \quad (24)$$

which vanishes again for $n=0$. It is nothing amazing in these results as well as the analogous results derived above about $n_r=0$. This means that in such cases inequality having a form with zero in r.-h.-s. does not impose any restriction for the values of variances besides the condition that there should be $0\le\Delta_{\phi}A<\infty$ and $0\le\Delta_{\phi}B<\infty$ .It is easy to demonstrate that in case of multidimensional central potentials the situation is similar to that of 3-dimensional one.

Summary and Conclusions

We have shown, that the average value of commutator of non-commuting operators is vanishing for some physical states. It will be not hardly surprising if no connection to the Heisenberg-Robertson relation. The point is that this commutator restricts the precision of measurement of corresponding observables. According to the common believe, if two operators do not commute, then the corresponding observables are not measurable quantities simultaneously. Our results show that there are examples, where even when operators do not commute, the Heisenberg-Robertson inequality does not give any limitation on relevant physical quantities. This contradicts to general principles of quantum mechanics. We hope that this discrepancy happens only in the approach, when the product of uncertainties is proportional to corresponding commutators. Therefore, by our opinion some distinguished approaches may be more suitable in this purpose. It is why many authors (see [11, 12]) considered other relations or modify HR, in order to include some additional terms for improving HR in the correct direction.

ფიზიკა

ჰაიზენბერგ-რობერტსონის განუზღვრელობის თანაფარდობის და კვანტური მექანიკის პრინციპების შესაძლო შეუთავსებლობის შესახებ

ა. ხელაშვილი* და თ. ნადარეიშვილი*,**

**აკადემიის წევრი, ივანე ჯავახიშვილის სახ. თბილისის სახელმწიფო უნივერსიტეტი, მაღალი ენერგიების ფიზიკის ინსტიტუტი, თბილისი, საქართველო*
***ივანე ჯავახიშვილის სახ. თბილისის სახელმწიფო უნივერსიტეტი, ზუსტ და საბუნებისმეტყველო მეცნიერებათა ფაკულტეტი, ფიზიკის დეპარტამენტი; მაღალი ენერგიების ფიზიკის ინსტიტუტი, თბილისი, საქართველო*

ჰაიზენბერგის განუზღვრელობათა პრინციპის თანახმად არაკომუტირებადი დამზერადობის გაზომვების განუზღვრელობათა ნამრავლი ქვემოდან შემოზღუდულია შესაბამისი ოპერა-ტორების კომუტატორების საშუალო მნიშვნელობით ნებისმიერ მდგომარეობაში. კვანტური მექანიკის თითქმის ყველა სახელმძღვანელოში ამ თანაფარდობას აქვს ზოგადი ფორმა, რომელიც დაადგინა რობერტსონმა. შევნიშნოთ, რომ, მიუხედავად თანაფარდობის უდიდესი მნიშვნელობისა, ის არაერთხელ გამხდარა კრიტიკის ობიექტი სამეცნიერო ლიტერატურაში. მიღებულია შედეგები, რომლებიც ეწინააღმდეგება ამ თანაფარდობას. წარმოდგენილი სტა-ტიის მიზანია მოიძებნოს ახალი შემთხვევები, როცა ზემოხსენებული თანაფარდობა მცდარია. განხილულია კულონის, მოდიფიცირებული კულონის და სინგულარული ოსცილატორის მაგალითები. ნაჩვენებია, რომ კომუტატორის საშუალო ხდება ნული, როცა საშუალოვდება სათანადო ტალღური ფუნქციებით.

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