SOME QUANTUM MECHANICAL RELATIONS IN CASE OF SINGULAR OPERATORS

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1. Introduction

The aim of this talk is to study some quantum mechanical theorems in polar spherical coordinates, when the area of **radial** varuable is not a **full space**.We will see that in most cases **problems arises** when the **operators** in the Schrodinger equation **are singular.**

2. Time derivative of mean values of operators

In quantum mechanics **derivative** of time-dependent operator $\hat{A}(t)$ is transferred from the corresponding **classical expression** according to **replacement** of the Poison bracket by quantum commutator **[1. Landau L D Lifshitz E M 1977 *Quantum Mechanics* (Oxford: Pergamon). 2. Messiah A. Two Volumes Bound as One, *Quantum Mechanics*, Dover Publications, 1999]**

$$\frac{d\hat{A}}{dt} = \frac{\partial \hat{A}}{\partial t} + \frac{i}{\hbar}\left[\hat{H}, \hat{A}\right] \qquad (2.1)$$

If one **averages** (2.1) by the state function, it follows

$$\left\langle \frac{d\hat{A}}{dt} \right\rangle = \left\langle \frac{\partial \hat{A}}{\partial t} \right\rangle + \frac{i}{\hbar}\left\langle \left[\hat{H}, \hat{A}\right] \right\rangle \qquad (2.2)$$

As a rule one **believes** that these two operations – time derivative and average procedures **can be interchanged**. This is **postulated as a definition** [1]

$$\left\langle \frac{d\hat{A}}{dt} \right\rangle = \frac{d\left\langle \hat{A} \right\rangle}{dt} = \left\langle \frac{\partial \hat{A}}{\partial t} \right\rangle + \frac{i}{\hbar}\left\langle \left[\hat{H}, \hat{A} \right] \right\rangle \qquad (2.3)$$

We show, that is not it true in general. The derivate is

$$\frac{d\left\langle \hat{A} \right\rangle}{dt} = \frac{d}{dt}\left\langle \psi \middle| \hat{A} \middle| \psi \right\rangle = \left\langle \frac{\partial \psi}{\partial t} \middle| \hat{A} \middle| \psi \right\rangle + \left\langle \psi \middle| \frac{\partial \hat{A}}{\partial t} \middle| \psi \right\rangle + \left\langle \psi \middle| \hat{A} \middle| \frac{\partial \psi}{\partial t} \right\rangle$$

(2.4)

If we use the **time dependent** Schrodinger eqation and its complex conjugate in the **first** and **third** terms of eq. (2.4) and take the Hamiltonian in the radial form

$$\hat{H} = \frac{1}{2m}\left(-\frac{d^2}{dr^2} - \frac{2}{r}\frac{d}{dr} \right) + \frac{l(l+1)}{2mr^2} + V(r,t) \qquad (2.5)$$

and **performing two-fold partial integration,** we get

$$\frac{d\left\langle \hat{A} \right\rangle}{dt} = \frac{i}{\hbar}\left\langle \left[\hat{H}, \hat{A} \right] \right\rangle + \left\langle \frac{\partial \hat{A}}{\partial t} \right\rangle + \Pi \qquad (2.6)$$

where we have obtained the **additional** term

$$\Pi = i\frac{\hbar}{2m}\lim_{r\to 0}\left\{r^2\left[\hat{A}R\frac{dR^*}{dr} - R^*\frac{d}{dr}(\hat{A}R)\right]\right\} \tag{2.7}$$

This term is **not zero in general**- it depends on the **behavior** of wave function and operator **at the origin.** It has **no classical analogue** ($\hbar \to 0$, (2.7) tends **to zero**)

It is known that under **general requirements** that

$$\underset{r\to 0}{rR(r)} = 0 \tag{2.8}$$

(See **[3. A.Khelashvili and T.Nadareishvili. Am. J. Phys. 79 668 (2011) 4. A. Khelashvili and T. Nadareishvili. European J.Phys 35 065026 (2014). 5. A.Khelashvili and T. Nadareishvili.Phys. of Particles and Nuclear Lett. 12, 11(2015).**The behavior depends on **potential**

- **Regular potentials:** They behave as

$$\lim_{r\to 0} r^2 V(r) = 0 \tag{2.9}$$

$$\underset{r\to 0}{R} \approx C_1 r^l \tag{2.10}$$

Satisfy (2.8) condition

- **"soft" singular potentials**, for which

$$r^2 V(r) \underset{r\to 0}{\to} \pm V_0, \qquad (V_0 = const > 0) \tag{2.11}$$

For (2.11) wave function behavior is **[3-5]:**

$$\lim_{r\to 0} R = a_{st} r^{-1/2+P} + a_{add} r^{-1/2-P} \equiv R_{st} + R_{add} \tag{2.12}$$

$$P = \sqrt{(l+1/2)^2 - 2mV_0} > 0 \tag{2.13}$$

For $0 < P < 1/2$ the **second** solution satisfies also **boundary condition** (2.8),so it must be **retained**. For $P \geq 1/2$ only the **first** solution **remains.**

Now consider of **additional contribution** in Eq. (2.6). Consider **regular** potentials. It is **clear** from Eq. (2.7) that the **singularity** of $\hat{A}$ at the **origin** will be also **important.**

$$\hat{A}(r) \sim \frac{1}{r^{\beta}}; \quad \beta > 0 \tag{2.14}$$

$$\Pi_{reg} = \frac{i\hbar C_1^2}{2m} \lim_{r\to 0} r^{2l+1-\beta} \tag{2.15}$$

In order (2.15) will not be **diverging** we must **require**

$$2l + 1 > \beta \tag{2.16}$$

For (2.16) **additional term vanishes**. In opposite case the **divergent** result follow- we are **unable** to write (2.2). For

$$2l+1=\beta \tag{2.17}$$

$$\frac{d\langle A\rangle}{dt}=\left\langle\frac{\partial\hat{A}}{\partial t}\right\rangle+\frac{i}{\hbar}\left\langle\left[\hat{H},\hat{A}\right]\right\rangle+\frac{i\hbar C_1}{m}\left(l+\frac{1}{2}\right) \tag{2.18}$$

So the averaging relation is **not so trivial** and is depends on **singularity of operator**.

For (2.12) for standard solution $R=R_{st}=a_{st}r^{-1/2+P}$:

$$\Pi_{st}=i\hbar\frac{a_{st}^2\beta}{2m}\lim_{r\to 0}r^{2P-\beta} \tag{2.19}$$

Here also we get $\Pi_{st}=0$ zero, when

$$2P>\beta \tag{2.20}$$

$$2P=\beta \tag{2.21}$$

$$\frac{d\langle\hat{A}\rangle}{dt}=\left\langle\frac{\partial\hat{A}}{\partial t}\right\rangle+\frac{i}{\hbar}\left\langle\left[\hat{H},\hat{A}\right]\right\rangle+\frac{i\hbar a_{st}^2}{m}P \tag{2.22}$$

Conclusion: The well-known averaging relation is validating only in cases, when the condition (2.16) and (2.20) is satisfied. This''strange'' result is provided **by singular character of the operator.** The **strangest** is the fact that the time derivative of average value **does not coincide** to the average of derivative of the operator

$$\left\langle \frac{d\hat{A}}{dt} \right\rangle = \frac{d\left\langle \hat{A} \right\rangle}{dt} - \Pi \tag{2.23}$$

We see that if the operator has **a "bad" singularity ((2.17) or (2.21)),** its average value **is not an integral of motion if it even commutes with the Hamiltonian. Morever, many famous theorems like Ehrenfest or hypervirial relations may be modified.[6. Z. Ehrenfest, Z.Phys,Vol.45, 455 (1927);7.O.Hirschfelder,J.Chem Physics. 33,1462 (1960)]**

3.Stationary states and integrals of motion

$$\psi(\boldsymbol{r},t) = e^{-\frac{i}{\hbar}Et}\phi(\boldsymbol{r}) \tag{3.1}$$

If $\hat{A}$ is not **explicitly dependent on time**, we should have

$$\left\langle \frac{d\hat{A}}{dt} \right\rangle = \left\langle \frac{i}{\hbar}\left[\hat{H},\hat{A}\right] \right\rangle, \tag{3.2}$$

$$\left\langle \frac{d\hat{A}}{dt} \right\rangle = \frac{i}{\hbar}\left\{ \int_0^\infty R^* HARr^2 dr - E\int_0^\infty R^* \hat{A}Rr^2 dr \right\} \tag{3.3}$$

Here we have use that ϕ is a eigenfunction of $\hat{H}$

Let us consider **two cases**:

(a). $\hat{A}$ commutes with $\hat{H}$. Then it follows

$$\left\langle \frac{d\hat{A}}{dt} \right\rangle = \frac{d\left\langle \hat{A} \right\rangle}{dt} = 0 \qquad (3.4)$$

So,for stationary state if time-independent $\hat{A}$, commutes with the Hamiltonian, in spite of its singular character, the relation (3.4) is valid, the mean value of this operator is conserved and is an integral of motion.

(b) $\hat{A}\hat{H} \neq \hat{H}\hat{A}$ Let study the integral entering (3.3)

$$I = \frac{i}{\hbar}\int_0^\infty R^* \hat{H}\hat{A} R r^2 dr \qquad (3.5)$$

$$I = \frac{i}{\hbar}\int_0^\infty \hat{H} R^* \hat{A} R r^2 dr - \Pi = \frac{i}{\hbar} E \int_0^\infty R^* A R r^2 dr - \Pi \qquad (3.6)$$

$$\left\langle \frac{d\hat{A}}{dt} \right\rangle = -\Pi \qquad (3.7)$$

When $\hat{A}$ is **independent on time**, we have

$$\langle A\rangle = \int e^{\frac{i}{\hbar}Et}\phi^*(\mathbf{r})\hat{A}e^{-\frac{i}{\hbar}Et}\phi(\mathbf{r})d^3\mathbf{r} = \int \phi^*(\mathbf{r})\hat{A}\phi(\mathbf{r})d^3\mathbf{r} \quad (3.8)$$

It is evident that

$$\frac{d\langle A\rangle}{dt} = 0 \quad (3.9)$$

We have obtained a ''*strange*'' result: for stationary states, for $\hat{A}\hat{H} \neq \hat{H}\hat{A}$, Eq. (3.9) is valid or $\langle \hat{A}\rangle$ is conserved, but according to Eq. (3.7) $\left\langle \frac{d\hat{A}}{dt}\right\rangle \neq 0$. In this particular case this 'strange" result is provided by singularity of operator $\hat{A}$. Therefore, we conclude from this result that the definition, given by Eq. (2.3), **depends on the singularity** of the operator. **Remark, that this point was not discussed in the literature up to now.**

SOME APPLICATIONS

4. Modified hypervirial theorems

Comparing Eqs. (3.2) and (3.7), one derives

$$\frac{i}{\hbar}\left\langle\left[\hat{H},\hat{A}\right]\right\rangle=-\Pi \tag{4.1}$$

So well-known hypervirial theorems should be corrected **[8.S.T.Epstein,O.Hirschfelder,Phys.Rev.123,1495(1961)]9.O.Hirschfelder,C.Coulson.J.Chem.Physics.36,941(1962)]** ***If*** ϕ ***is a bound state eigenfunction of a Hamiltonian*** $\hat{H}$ ***and if*** $\hat{A}$ ***is an arbitrary Hermitian time-independent operator involving the coordinates and momenta, then hypervirial theorem for*** $\hat{A}$ ***states that***

$$\left\langle\phi,\left[\hat{H},\hat{A}\right]\phi\right\rangle=0 \tag{4.2}$$

(4.2) must be **modified** and according to Eq. (4.1):

$$\left\langle\phi,\left[\hat{H},\hat{A}\right]\phi\right\rangle=i\hbar\Pi \tag{4.3}$$

- Some applications of the (4.3). For [8]

$$A=\hat{p}_r r^{S+1} \tag{4.4}$$

$$\hat{p}_r=\frac{\hbar}{i}\left(\frac{\partial}{\partial r}+\frac{1}{r}\right) \tag{4.5}$$

From Eqs. (2.8) and (2.13) that for **standard** solutions

$$\Pi_{st} = -\frac{\hbar^2 a_{st}^2}{2m} S\left(P + S + \frac{3}{2}\right)\lim_{r\to 0} r^{2P+S} \tag{4.6}$$

If $2P > -S$, then $\Pi_{st} = 0$, but when $2P = -S$, then

$$\Pi_{st} = -\frac{\hbar^2 a_{st}^2}{4m} S(S+3) \tag{4.7}$$

For $2P < -S$, Π_{st} **diverges**, or in this case the **hypervirial theorem does not work.**

For regular potentials when $P = l + \frac{1}{2}$

$$\Pi_{reg,l} = \frac{\hbar C_l^2}{2m}(2l+1)(1-l)\lim_{r\to 0} r^{2l+S+1} \tag{4.8}$$

Which survives, if $S = -(2l+1)$. In this case

$$\Pi_{reg,l} = \frac{\hbar^2 C_l^2}{2m}(2l+1)(1-l) \tag{4.9}$$

So the **modified hypervirial theorems** for the Coulomb $V = -\frac{e^2}{r}$ and oscillator potentials $V = \frac{m}{2}\omega^2 r^2$ have the forms

$$2E(s+1)\langle r^{s}\rangle + e^{2}(2s+1)\langle r^{s-1}\rangle + \frac{s\hbar^{2}}{4m}\left[s^{2}-(2l+1)^{2}\right]\langle r^{s-2}\rangle = -\frac{\hbar^{2}}{2m}(2l+1)^{2}C_{l}^{2}\delta_{S+1,-2l}$$
(4.10)

$$2E(s+1)\langle r^{s}\rangle - m\omega^{2}(s+2)\langle r^{s+2}\rangle + \frac{s\hbar^{2}}{4m}\left[s^{2}-(2l+1)^{2}\right]\langle r^{s-2}\rangle = -\frac{\hbar^{2}}{2m}(2l+1)^{2}C_{l}^{2}\delta_{S+1,-2l}$$
(4.11)

Where $C_{l} = \lim_{r\to 0} r^{-l}R_{l}(r)$

5. Modification of the Ehrenfest theorem

If the operator of radial momentum

$$\hat{A} = \hat{p}_{r} = \frac{\hbar}{i}\left(\frac{\partial}{\partial r} + \frac{1}{r}\right) \qquad (5.1)$$

substitute into Eq. (2.6), we obtain

$$\frac{d\langle \hat{p}_{r}\rangle}{dt} = \frac{i}{\hbar}\left\langle\left[\hat{H}, \hat{p}_{r}\right]\right\rangle + \Pi_{st} \qquad (5.2)$$

$$\Pi_{st} = \frac{a_{st}^{2}\hbar^{2}}{2m}\left(\frac{1}{2}+P\right)\lim_{r\to 0} r^{2P-1} \qquad (5.3)$$

For $2P > 1$ $\Pi_{st} = 0$, while for $2P < 1$, it **diverges.**
But for $2P = 1$ it **survives**

$$\Pi_{st} = \frac{a_{st}^2 \hbar^2}{2m} \qquad (5.4)$$

So for **singular** potential the usual Ehrenfest theorem

$$\frac{d\langle \hat{p}_r \rangle}{dt} = \frac{i}{\hbar}\left\langle \left[\hat{H}, \hat{p}_r\right]\right\rangle \qquad (5.5)$$

is applicable only **in the first case** $2P > 1$. In other cases the **additional term (5.4) appears** or has not place at all. **In the traditional textbooks this fact is not mentioned.**

$$\left[\hat{H}, \hat{p}_r\right] = -i\frac{\hbar^2 l(l+1)}{mr^3} - i\hbar F_r \qquad (5.6)$$

F_r is a radial force. Ehrenfest **modified theorem**

$$\frac{d\langle p_r \rangle}{dt} = \frac{\hbar l(l+1)}{m}\left\langle \frac{1}{r^3}\right\rangle + \langle F_r \rangle + \Pi_{st} \qquad (5.7)$$

This relation is a new one.

For regular potentials $P = l + 1/2$, only in case $l > 0$ it follows $\Pi_{reg} = 0$. **But** for $l = 0$ **we have**

$$\Pi_{reg} = \frac{C_0^2 \hbar^2}{2m} \qquad (5.8)$$

So for **regular** potentials the usual Ehrenfest theorem is **valid only in the case** $l > 0$, but for $l = 0$ there appears an **extra term** (5.8).

Now let us show that Eq. (5.7) gives **correct** results for **Coulomb** potential.

$l > 0$. In this case $\Pi_{reg} = 0$. In **[10.U.Roy. Arxiv:0704.0373.(2007).11.U.Roy.Arxiv:0706.0924.(2008).]** right-hand side of theorem consist only forces $\frac{\hbar l(l+1)}{m}\left\langle\frac{1}{r^3}\right\rangle + \langle F_r\rangle$: two forces **compensate each other.**

$l = 0$ is **more interesting.** We have **no centrifugal term**, the additional term is given by (5.8),

$$\frac{d\langle p_r\rangle}{dt} = \langle F_r\rangle + \frac{C_0^2\hbar^2}{2m} \qquad (5.9)$$

$$\langle F_r\rangle = -\frac{2e^2}{n^3 a_0^2} \qquad (5.10)$$

In stationary case the left-hand side of (5.10) must **be zero**. So we should have

$$\frac{C_1^2\hbar^2}{2m}=\frac{2e^2}{n^3a_0^2} \tag{5.11}$$

And it follows a **correct** expression for Bohr's first orbit radius $a_0=\dfrac{\hbar^2}{me^2}$

We conclude that in Eq. (5.7) the term Π_{st} must present necessarily for deriving correct results, which is absent in [10-11]. For $\hat{A}=\hat{r}$ we find

$$\Pi_{st}=-i\frac{a_{st}^2\hbar^2}{2m}\lim_{r\to 0}r^{2P+1}=0 \tag{5.12}$$

because $P>0$. It vanishes also for **regular** potentials, because for them $P=l+1/2>0$. So

$$\frac{d\langle\hat{r}\rangle}{dt}=\frac{i}{\hbar}\left\langle\left[\hat{H},\hat{r}\right]\right\rangle \tag{5.13}$$

both for regular as well as singular potentials

$$\frac{d\langle\hat{r}\rangle}{dt}=\frac{\langle p_r\rangle}{m} \tag{5.14}$$

The obtained results are **understandable,** because the momentum operator is **singular at the origin** in spite of the coordinate operator.

6. Conclusions

1) We considered an **influence of the restricted region** in 3-dimensional space in the ordinary quantum mechanics, where the radial wave function is defined on a **semi-space.** Therefore the boundary behavior of radial function **contributes to the several fundamental relations.** The **additional contributions appear** also from **singular behavior** of operators. **The last fact was not discussed earlier.**

2) We derived the explicit algorithm of **calculation of this extra term** and investigated conditions, when it **changes** fundamental relations.

3) Application to several known problems shows that the **inclusion of the extra term is necessary** in order to avoid some misunderstandings.

We believe that the above developed formalism should have many other application also, especially, in derivation of **uncertainty relations.**

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Thank you for attention!