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Physics

Hermiticity of Physical Operators in Spherical Coordinates

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It is well known that that for the unbounded operators, corresponding to the quantum observables, it is necessary to specify the class of functions (called domain), on which they are defined. Less attention is allocated to this fact in teaching books. Especially it deals with self-adjoint operators, spectral properties of which are essential for describing the physical systems. It should be noted that before the attention mainly was dedicated to one-dimensional problems in the limited areas, where the boundary conditions came into play. In the paper we take an attention to the fact, that in case of spherical symmetry in the Schrodinger equation after a separation of variables the dynamics is described by the radial equations, which are one dimensional, but the radial variable is restricted from one side from the beginning. Therefore, their solutions, the radial functions, have to satisfy to certain boundary conditions at the origin of coordinates. Furthermore, operators' singularity to be also taken into account.

Spherical coordinates, Hermitian operators, Schrodinger equation

Proper quantization of physical systems requires correct definition of physical variables (such as the Hamiltonian, momentum, etc.,) as self-adjoint operators in an appropriate Hilbert space and their spectral analysis [1]. Observables are usually presented as hermitian operators (matrices). They have important properties like real eigenvalues, the corresponding eigenvectors are orthogonal and span the whole finite dimensional Hilbert space, etc. However, all this properties are not ensured by the hermiticity condition in general infinite-dimensional Hilbert space. Hermiticity condition is often just replaced with the symmetricity condition, which only ensures for the expectation values of observables to be real [2], while the rest of the properties can only be grasped with imposing the more subtle condition called self-adjointness.

A crucial subtlety is that an unbounded self-adjoint operator cannot be defined in the whole Hilbert space, i.e. on an arbitrary quantum mechanical state [3].

In the textbooks on quantum mechanics most formulations concern mainly one-dimensional problems, in these cases, and as a rule, wave functions decrease at both infinity (Hilbert space). Mostly the problems in full infinite space are considered. However, as is well known, when system is localized in finite volume, the inclusion of boundary conditions becomes necessary as well as they impose the restrictions on the allowed classes of wave functions [4].

This problem often arises in many-dimensional ($N \geq 3$) cases, when the polar (spherical) coordinates are necessarily introduced, because the radial functions are defined in semi-line. In such cases problems with restricted area emerge automatically.

In case of spherical symmetry in the Schrodinger equation variables are separated in spherical coordinates and all dynamics is concentrated into the radial equation, which contains only a radial distance r. The problem is reduced to one-dimensional case, but on the half-line. It means that we have to deal with restricted area. Therefore, the boundary conditions at the origin come into play. Moreover, there appear two one-dimensional equations, one – for total radial function, $R(r)$, and the second – for the reduced wave function, $u(r) = rR(r)$. They obey to different boundary conditions, therefore one and the same operator may have different hermiticity properties.

Below this question is discussed and corresponding statements are derived. Let us begin with known definitions: The operator $\hat{A}$ is Hermitian (symmetric), if it obeys to the following condition

$$\left\langle \hat{A}\psi \middle| \varphi \right\rangle = \left\langle \psi \middle| \hat{A}\varphi \right\rangle \tag{1}$$

where ψ and φ are squared integrable functions, decaying at infinity. Bearing in mind that operators can contain a differentiation, we expect that a possible extra contribution can appear after the partial integration.

Consider specific examples:

$$1. \quad \hat{A} = -i\hbar \frac{\partial}{\partial r} \tag{2}$$

We obtain

$$\begin{gathered} \left\langle \hat{A}R \middle| R \right\rangle = i\hbar \int_0^\infty \left(\frac{\partial R}{\partial r} \right)^* Rr^2 dr = \left(i\hbar \left\{ \left[R^* Rr^2 \right]_0^\infty - \int_0^\infty R^* \frac{\partial \left(Rr^2 \right)}{\partial r} dr \right\} \right) = \\ = -i\hbar \left\{ \int_0^\infty R^* \left\{ \left[\frac{2}{r} + \frac{\partial}{\partial r} \right] R \right\} r^2 dr \right\} = -2i\hbar \int_0^\infty R^* R r dr - i\hbar \int_0^\infty R^* \left(\frac{\partial R}{\partial r} \right) r^2 dr \neq \left\langle R \middle| AR \right\rangle. \end{gathered} \tag{3}$$

Here, in the first row we made use of the well-known boundary and normalization conditions [5]

$$\lim_{r \to 0} rR = u(0) = 0 \,, \ \int_0^\infty R^* R r^2 dr = 1. \tag{4}$$

We see, that the Hermiticity condition (1) in equation (3) is not satisfied and the operator (2) is not Hermitian in the domain of $R(r)$ functions, i.e., functions from the Hilbert space, obeying to the additional conditions (4). On the other hand, for the reduced radial functions $u(r)$ this operator becomes Hermitian. Indeed:

$$\begin{gathered} \left\langle \hat{A}u \middle| u \right\rangle = (-i\hbar) \int_0^\infty \left(\frac{\partial u}{\partial r} \right)^* u dr = (-i\hbar) \left\{ \left[u^* u \right]_0^\infty - \int_0^\infty u^* \left(\frac{\partial u}{\partial r} \right) dr \right\} = \\ = (-i\hbar) \left\{ -\int_0^\infty u^* \left(\frac{\partial u}{\partial r} dr \right) \right\} = i\hbar \int_0^\infty u^* \frac{\partial u}{\partial r} dr = \left\langle u \middle| \hat{A}u \right\rangle. \end{gathered} \tag{5}$$

Therefore, the considered operator is Hermitian in the domain of reduced functions, $u(r)$. It is not surprising, because there is no operator without its domain of definition: operators are defined not only by their action (i.e. what they do to the functions on which they operate), but also by their domain [3] (that is, the set of functions on which they operate).

2. Consider now the radial momentum operator [4]

$$\hat{p}_r = -i\hbar\left(\frac{\partial}{\partial r}+\frac{1}{r}\right) \tag{6}$$

Let us verify that $\langle \hat{p}_r\psi|\varphi\rangle = \langle\psi|\hat{p}_r\varphi\rangle$. We have

$$\langle \hat{p}_r R|R\rangle = i\hbar\int_0^\infty\left(\frac{\partial}{\partial r}+\frac{1}{r}\right)R^*Rr^2dr = i\hbar\left\{\int_0^\infty\left(\frac{\partial R^*}{\partial r}\right)Rr^2dr+\int_0^\infty\frac{1}{r}R^*Rr^2dr=\right\}$$

$$= i\hbar\left\{\left[R^*Rr^2\right]_0^\infty - \int_0^\infty R^*\left(\frac{\partial\left(Rr^2\right)}{\partial r}\right)dr+\int_0^\infty\frac{1}{r}R^*Rr^2dr\right\}=$$

$$= i\hbar\left\{-\int_0^\infty R^*\left(rR+\frac{\partial R}{\partial r}r^*\right)dr\right\} = -i\hbar\int_0^\infty R^*\left\{\left(\frac{\partial}{\partial r}+\frac{1}{r}\right)R\right\}r^2dr = \langle R|\hat{p}_r R\rangle. \tag{7}$$

Therefore,the operator (6) is Hermitian on the class of radial functions R , satisfying to (4).

Note, that on the domain of reduced radial functions $u(r)$ this operator is not Hermitian. Indeed:

$$\langle \hat{p}_r u|u\rangle = i\hbar\int_0^\infty\left(\frac{\partial}{\partial r}+\frac{1}{r}\right)u^*udr = i\hbar\left\{\int_0^\infty\left(\frac{\partial u^*}{\partial r}\right)udr+\int_0^\infty\frac{1}{r}u^*udr\right\}=$$

$$= i\hbar\left\{u^*u\Big|_0^\infty - \int_0^\infty u^*\left(\frac{\partial u}{\partial r}\right)dr+\int_0^\infty\frac{1}{r}u^*udr\right\} = i\hbar\left\{-\int_0^\infty u^*\frac{\partial u}{\partial r}dr+\int_0^\infty\frac{1}{r}u^*udr\right\}$$

$$= -i\hbar\left\{\int_{00}^\infty u^*\frac{\partial u}{\partial r}dr-\int_0^\infty\frac{1}{r}u^*udr\right\} = -i\hbar\int_0^\infty u^*\left(\frac{\partial}{\partial r}-\frac{1}{r}\right)udr \neq \langle u|\hat{p}_r u\rangle. \tag{8}$$

Therefore $\hat{p}_r$ is not Hermitian on the space of $u(r)$ functions. The same is proven in [5]

Moreover, this operator is not an observable, i.e. its eigenvalues are not real. Indeed, for any constant number ω, the solution of differential equation

$$\hat{p}_r f(r) = \omega f(r) \tag{9}$$

up to constant number is $\exp(i\omega r/\hbar)/r$. This solution does not obey to the boundary condition (4), the eigenvalue problem satisfying to (4) does not exist. This operator is hermitian (symmetric) on the functions from (4), but its extension up to self-adjoint is impossible (See L.Faddeev’s comment from the book of A. Messhia [4]).

In many applications of the Heisenberg-Robertson uncertainty relation various commutators appear on the right-hand side of operators’ uncertainties product. In spherical symmetry problem the following commutator is of particular interest

$$\left[r^2, p^2\right] \equiv \hat{C} = -4\hbar^2\left(r\frac{d}{dr}+\frac{3}{2}\right). \tag{10}$$

It is an easy exercise to show, that the operator in the right side is Hermitian on the functions, obeying condition (4), i.e.

$$\left\langle \hat{C}R \middle| R \right\rangle = \left\langle R \middle| \hat{C}R \right\rangle. \tag{11}$$

In fact, explicit calculation goes as follows

$$\left\langle \hat{C}R \middle| R \right\rangle = \int_0^\infty \left(\hat{C}R\right)^* Rr^2 dr = 4i\hbar^2 \int_0^\infty \left\{ \left(r\frac{\partial}{\partial r} + \frac{3}{2} \right) R^* \right\} Rr^2 dr =$$

$$= 4i\hbar^2 \left\{ \frac{3}{2} + \int_0^\infty r\frac{\partial R^*}{\partial r} Rr^2 dr \right\} = 4i\hbar^2 \left\{ \frac{3}{2} + \left[R^* R r^3 \right]_0 - \int_0^\infty R^* \frac{\partial\left(Rr^3\right)}{\partial r} dr \right\} =$$

$$= 4i\hbar^2 \left\{ \frac{3}{2} - \int_0^\infty R^* \left(3r^2 R + \frac{\partial R}{\partial r} r^3 \right) dr \right\} = -4i\hbar^2 \left\{ \frac{3}{2} + \int_0^\infty R^* \frac{\partial R}{\partial r} r^3 dr \right\}. \tag{12}$$

On the other hand, the right-side is

$$\left\langle R \middle| \hat{C}R \right\rangle = -4i\hbar^2 \int_0^\infty R^* \left(r\frac{\partial}{\partial r} + \frac{3}{2} \right) Rr^2 dr = -4i\hbar^2 \left\{ \frac{3}{2} + \int_0^\infty R^* \frac{\partial R}{\partial r} r^3 dr \right\}, \tag{13}$$

which exactly coincides to previous result. In addition, we made use of normalization condition $\left\langle R \middle| R \right\rangle \equiv \int_0^\infty R^* R r^2 dr = 1$. Therefore, condition (9) is fulfilled and the operator (8) is Hermitian on domain of $R(r)$ functions.

On the other hand, this equality is violated on the domain of $u(r)$ functions.

Consider now the operator p^2, which stands in the left-hand side of Eq.(8) and check its hermiticity property

$$\left\langle p^2 R \middle| R \right\rangle = \left\langle R \middle| p^2 R \right\rangle. \tag{14}$$

Using the Schrodinger equation, we substitute

$$p^2 = 2m\left(H - V\right) = \left(p_r^2 + \frac{\hbar^2 l\left(l+1\right)}{r^2} \right) = \hbar^2 \left[-\frac{d^2}{dr^2} - \frac{2}{r}\frac{d}{dr} + \frac{\hbar^2 l\left(l+1\right)}{r^2} \right], \tag{15}$$

therefore

$$\frac{1}{2m}\left\langle p^2 R \middle| R \right\rangle = \frac{1}{2m}\int_0^\infty \left(p^2 R\right)^* Rr^2 dr = \int_0^\infty \left[\left(H - V\right)R\right]^* Rr^2 dr. \tag{16}$$

Consider the first term under the integral and use the relation from our work [6]

$$\int_0^\infty \left[HR\right]^* ARr^2 dr = \int_0^\infty R^* HARr^2 dr + \Pi, \tag{17}$$

where

$$\Pi = i\frac{\hbar^2}{2m}\lim_{r\to 0}\left\{ r^2 \left[\hat{A}R\frac{\partial R^*}{\partial r} - R^* \frac{\partial}{\partial r}\left(\hat{A}R\right) \right] \right\}. \tag{18}$$

If we take here $\hat{A} = I$, the additional term disappears and Eq. (16) gives (because $V(r)$ is simply a multiplication operator)

$$\frac{1}{2m}\left\langle p^2 R \middle| R \right\rangle = \int_0^\infty \int_0^\infty \left[(H - V) R \right]^* R r^2 dr = \frac{1}{2m} \left\langle R \middle| p^2 R \right\rangle. \tag{19}$$

Hence, we conclude that p^2 is a Hermitian operator on functions $R(r)$.

On the other hand, on reduced functions $u(r)$ this operator behaves as

$$\frac{1}{2m}\int_0^\infty \left(p^2 u \right)^* u dr = \int_0^\infty \left[(H - V) u \right]^* u dr = \int_0^\infty \left[Hu \right]^* \hat{A} u dr + \Pi, \tag{20}$$

where

$$\Pi = i\frac{\hbar^2}{2m}\lim_{r\to 0}\left\{ \left[\hat{A}u \frac{\partial u^*}{\partial r} - u^* \frac{\partial}{\partial r}\left(\hat{A}u \right) \right] \right\}. \tag{21}$$

Taken here $\hat{A} = I$, as before, the additional term disappears, and we find

$$\left\langle p^2 u \middle| u \right\rangle = \int_0^\infty \left[(H - V) u \right]^* u dr = \left\langle u \middle| p^2 u \right\rangle. \tag{22}$$

Therefore, even in space of $u(r)$ with the boundary condition (4) the operator p^2 is Hermitian.

ფიზიკა

ფიზიკური ოპერატორების ჰერმიტულობა სფერულ კოორდინატებში

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ცნობილია, რომ შემოუსაზღვრელი ოპერატორებისთვის, როგორიცაა კვანტური მექანიკის ფიზიკური ოპერატორები, აუცილებელია მითითებულ იქნეს ფუნქციათა კლასი, რომელზეც ისინი არიან განმარტებული. სახელმძღვანელოებში ამ ფაქტს ნაკლები ყურადღება აქვს მიქცეული. განსაკუთრებით, ეს ეხება თვითშეუღლებულ ოპერატორებს, რომელთა სპექტრალური თვისებები არსებითია ფიზიკური სისტემის აღწერისათვის. უნდა აღინიშნოს, რომ უკანასკნელი პერიოდის ნაშრომებში მთავარი ყურადღება ექცევა ერთგანზომილებიან ამოცანებს შეზღუდულ არეებში, რომლებისთვისაც საჭირო ხდება სასაზღვრო პირობების მითითება ფუნქციათა არეების დასადგენად. წინამდებარე ნაშრომში ყურადღებას ვაქცევთ იმ გარემოებას, რომ სფერული სიმეტრიის დროს შრედინგერის განტოლებაში ცვლადთა განცალების შემდეგ მიიღება დინამიკის აღმწერი რადიალური განტოლება, რომელიც არის ერთგანზომილებიანი, ოღონდ რადიალური ცვლადი თავიდანვე შეზღუდულია ცალმხრივად. ამიტომ მისმა ამონახსნმა – რადიალურმა ფუნქციამ – უნდა შეასრულოს გარკვეული სასაზღვრო პირობა სათავეში. ამავე დროს შეზღუდვები ეხება თვით ოპერატორების სინგულარულ თვისებებსაც.

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