Singularity of the Laplace Operator in spherical coordinates and some of its consequences for the Radial Schrodinger Equation

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1. Introduction

It is well-known that a radial part of the Laplace operator in spherical coordinates has the form [1]

$$\Delta_r = \frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr} \quad (1)$$

This form often is written in two alternative compact expressions

$$\Delta_1 = \frac{1}{r^2}\frac{d}{dr}\left(r^2 \frac{d}{dr}\right) \quad (2)$$

or

$$\Delta_2 = \frac{1}{r}\frac{d^2}{dr^2}(r \quad) \quad (3)$$

It is easy to check by direct inspection that these two operator expressions are equal to each others and that of (1):

$$\Delta_1 = \Delta_2 = \Delta_r \quad (4)$$

There arise a natural question - are these equalities valid at the origin, $r = 0$?

The matter is that, spherical coordinates are defined when $r > 0$. But in most applications in physics the point $r = 0$ is an ordinary point, where the knowledge of behavior of physical quantities is necessary.

Below we show that this equality breaks down at origin. This result is absolutely new and unexpected by our knowledge.

First of all, let us remember what this equality means in quantum mechanics, i. e. in the Schrodinger equation. It is obvious that their action on on the full radial function $R(r)$ gives

$$\Delta_1 R(r) = \frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{d}{dr}\right)R = \frac{d^2R}{dr^2} + \frac{2}{r}\frac{dR}{dr} \tag{5a}$$

$$\Delta_2 R(r) = \frac{1}{r}\frac{d^2}{dr^2}(rR) \tag{5b}$$

Usually a new function, called radial wave function, is used to define (See for example [2])

$$u = rR \tag{6}$$

Therefore according to Eq. (5b), the equation for the new function $u(r)$ consists only the second derivative. This procedure has a wide application in quantum mechanics.
Now we show that this fact is correct only in special circumstances, depending on the boundary behavior of the radial wave function.

2. Appearance of singularity

Let us see what happens if this (6) radial function is substituted into the left hand-side also i.e. let us consider the equation $\Delta_r(R) = \Delta_r\left(\frac{u}{r}\right)$. We have

$$\frac{1}{r}\Delta_r(u) + u\Delta_r\left(\frac{1}{r}\right) + 2\frac{du}{dr}\frac{d}{dr}\left(\frac{1}{r}\right) = \frac{1}{r}\frac{d^2u}{dr^2} + \frac{2}{r^2}\frac{du}{dr} + u\Delta_r\left(\frac{1}{r}\right) - \frac{2}{r^2}\frac{du}{dr} \tag{7}$$

The last term cancels the first derivative term and, therefore, we are faced to the relation

$$\frac{1}{r}\frac{d^2u}{dr^2} + u\Delta_r\left(\frac{1}{r}\right) = \frac{1}{r}\frac{d^2u}{dr^2} - 4\pi\delta^{(3)}(\vec{\mathrm{r}})u((r) \tag{8}$$

Here we use well known relation [3]

$$\Delta_r\left(\frac{1}{r}\right) = \Delta\left(\frac{1}{r}\right) = -4\pi\delta^{(3)}(\vec{\mathrm{r}}) \tag{9}$$

We see that there appears an extra term, which is proportional to the Dirac's 3-dimensional delta function. This term was unnoted up to now. This term disappears when the origin $r = 0$ is excluded. Hence we have proved that above mentioned compact operator relations must be changed when the origin is included, probably as follows

$$\Delta_1 = \Delta_r = \Delta_2 - 4\pi\delta^{(3)}(\boldsymbol{r}) \qquad \textbf{(10)}$$

Comment: the form (10) is correct when we apply both sides on $u(r)$, but in case of R(r) it is necessary to change $\delta^{(3)}(\boldsymbol{r}) \rightarrow r\delta^{(3)}(\boldsymbol{r})$

3. Consequences

Rigorous consideration, demonstrated above shows that the radial wave function must be obtained from the following equation [4 - 5]

$$\frac{1}{r}\left[\frac{d^2u(r)}{dr^2} - \frac{l(l+1)}{r^2}u(r)\right] - 4\pi\delta^{(3)}(\vec{r})u(r) + 2m[E - V(r)]\frac{u(r)}{r} = 0 \qquad \textbf{(11)}$$

instead of the traditional form [See, e.g. any textbooks on quantum mechanics]

$$\frac{d^2u(r)}{dr^2} - \frac{l(l+1)}{r^2}u(r) + 2m\left[E - V(r)\right]u(r) = 0 \qquad \textbf{(12)}$$

Just this equation plays an important role in quantum mechanics since its birth.

Many problems with central potentials were solved on the basis of this equation. Last several decades many papers were devoted to the problems of a self-adjoint extension of the so-called radial Hamiltonian for singular potentials, based on this equation[6 - 7].Therefore it seems essential to make eq. (11) compatible with eq.(12) by neutralizing this extra delta function term.

It is clear beforehand that some boundary restriction at the origin on the radial wave function will appear owing to the properties of delta function. Indeed, the effect of three-dimensional delta function is determined by integrating over three dimensional volume element $d^3\boldsymbol{r} = r^2 dr \sin\theta d\theta d\varphi$. It is known that [3] $\delta^{(3)}(\boldsymbol{r}) = \frac{1}{|J|}\delta(r)\delta(\theta)\delta(\varphi)$, where $J = r^2\sin\theta$ is the Jacobian of transition to spherical coordinates. Thus, the extra term effectively acts as

$$u(r)\delta^{(3)}(\vec{r})d^3\vec{r} \rightarrow u(r)\delta(r)dr \qquad \textbf{(13)}$$

Therefore this extra term is equivalent to a point like source at $r = 0$, interacting with the wave function. Evidently this is physically nonsense. So the only reasonable way to remove this term requires that

$$u(0) = 0 \qquad \textbf{(14)}$$

Multiplication of eq. (11) on r and elimination of the delta function term due to property $r\delta(r)=0$ is not acceptable, because it is equivalent to multiplication of this term by zero. Therefore we must conclude that the radial equation (11) is compatible with the full Schrodinger equation

$$\Delta\psi(\vec{r})+2m[E-V(r)]\psi(\vec{r})=0 \qquad \textbf{(15)}$$

if and only if the supplementary condition (14) is satisfied. Moreover, to kill this delta function it is necessary that the degree of tending to zero at the origin of $u(r)$ be no less than 1.

It is remarkable to note that many authors, exploring the radial Hamiltonian

$$H_r \equiv -\frac{d^2}{dr^2}+\frac{l(l+1)}{r^2}+2mV(r) \qquad \textbf{(16)}$$

do not pay attention on the behaviour of radial wave function at the origin and content themselves by consideration only a square integrability of this function [6,7]. Of course, this is permissible mathematically and the strong theory of linear differential operators allows for such an approach [8-10]. There appears so-called Self-Adjoint Extended (SAE) physics [6], in the framework of which among physically reasonable solutions one encounters also many curious results, such as bound states in case of repulsive potential [7] and so on. We think that these highly unphysical results are caused by the fact that without suitable boundary condition at the origin a functional domain for radial Schrodinger Hamiltonian (16) is not restricted correctly. As we have seen above, Eq. (16) is a physical Hamiltonian and Eq. (12) is correct only if $u(0)=0$. To elucidate more clearly the points discussed above, let us investigate the eq. (11) near the origin carefully.

We said that for killing this extra delta term some specific behavior of the function $u(r)$ at the origin is necessary. In particular, if we take

$$u(r)_{r\to 0}\approx r^s \qquad \textbf{(17)}$$

,

we must require that $s\geq 1$[11-12]

It is remarkable to realize that the fact of appearing this delta function term does not depend on whether the potential is regular or singular. Behavior of potential at

$r \to 0$ **determines only a specific way of tending** $u(r)$ **to zero. Indeed, one can extract** $u(0)$ **from the true equation (11) in case of general behaved potential**

$$V(r)_{r\to 0} \approx \frac{g}{r^n}, \qquad (18)$$

Simple way consists in using the well- known representation for 3-dimensional delta-function (see, e.g. [13]).
in spherical coordinates:

$$\delta^{(3)}(\vec{r}) = \frac{1}{2\pi r^2}\delta(r) \text{ or } \delta^{(3)}(\vec{r}) = \frac{1}{4\pi r^2}\delta(r), \qquad (19)$$

depending on the definition of so-called sign-function at the origin. For our aims this difference is unessential. For definiteness we use below the second form. Then the Eq. (11) becomes:

$$\frac{1}{r}\left[\frac{d^2u(r)}{dr^2} - \frac{l(l+1)}{r^2}u(r)\right] - \frac{\delta(r)}{r^2}u(r) + +2m[E - V(r)]\frac{u(r)}{r} = 0 \qquad (20)$$

We must integrate this equation by the rest variable $r^2 dr$ **in a sphere of small radius** a **, tending it to zero after calculation. It gives**

$$\int_0^a r\frac{d^2u(r)}{dr^2}dr - l(l+1)\int_0^a \frac{u(r)}{r}dr - u(0) + \int_0^a (2mE - V(r))\frac{u(r)}{r}r^2 dr = 0 \qquad (21)$$

From this equation we determine

$$u(0) = \int_0^a r\frac{d^2u(r)}{dr^2}dr - l(l+1)\int_0^a \frac{u(r)}{r}dr + \int_0^a (2mE - V(r))u(r)r dr = 0 \qquad (22)$$

Because of smallness of radius a**, we can substitute here asymptotic form of the wave function at the origin in the form (17) and simultaneously, choose the potential at the origin in the form (18).**
Then, integration is easily performed and it follows:

$$u(0) = \left[\frac{s(s-1) - l(l+1)}{s}r^s + \frac{2mE}{s+2}r^{s+2} - \frac{2mg}{s+2-n}r^{s+2-n}\right]_0^a \qquad (23)$$

The elimination of this term from the Eq. (21) is necessary; otherwise we do not reach to the usual form of the radial equation (12). If it remains in equation, only three values are possible for it:

$u(0) = 0;$ $u(0)$ **is finite, or** $u(0)$ **is infinite**
(24)

Among them only the first case is acceptable, because the second value contradicts to the full Schrodinger equation, as far as $R(r)$ then behaves like $R(r) \approx \frac{const}{r}$ at the origin and it is not a solution of the full Schrodinger equation, because after it's substitution there appears again a new delta function. The third value is physically nonsense, because in this case we would have an infinite term in equation. **.**
Therefore, there remains only one reasonable value (14).

This boundary constraint must be fulfilled whether potential is regular or singular. Singular character of potential defines only the degree of turning of the wave function to zero. This follows from limiting equation (23), because all indices of exponents in this condition must be positive in order to provide vanishing of $u(0)$. So, the last exponent gives the relationship

$$s + 2 - n > 0 \qquad \textbf{(25)}$$

We see that, the growing the degree of singularity n, causes the growing of the decreasing exponent s of the wave function at the origin. Moreover, as $s \geq 1$, the radial wave function at the origin needs to be sufficiently regular. This fact may have far-reaching consequences.

4. Some applications

What does this result mean?

We take $s \geq 1$ and consider the radial equation (12) which is valid in this case. Let now discuss various potentials:

(1) Regular potentials:

$$\lim_{r \to 0} r^2 V(r) = 0 \qquad \textbf{(26)}$$

In this case the characteristic equation takes the form $s(s-1) = l(l+1)$, which gives two solutions

$$\underset{r \to 0}{u} \sim c_1 r^{l+1} + c_2 r^{-l} \qquad \textbf{(27)}$$

It follows that we must retain only the first one in (27), because $s_1 = l + 1 \geq 1$ and $s_2 = -l < 0$ Even in case of $l = 0$, nevertheless this $\underset{r \to 0}{u} \sim c_2 r^{-l}$ term does not destroy normalization of wave function near the origin, simply it is not a solution of full (15) Schrodinger equation.

Conclusion: In the case of regular potentials Eq.(12) is true radial equation and all results, obtained earlier on the basis of it, are correct!

(2) Consider now a slight generalization – singular transition potential

$$\lim_{r \to 0} r^2 V(r) = -V_0 = const \qquad \textbf{(28)}$$

Here $V_0 > 0$ corresponds to the attraction, while $V_0 < 0$ - to repulsion. Now Eq.(12) gives the following behavior at origin

$$\underset{r\to 0}{u} \sim d_1 r^{\frac{1}{2}+P} + d_2 r^{\frac{1}{2}-P} \ ; \ P = \sqrt{\left(l+\frac{1}{2}\right)^2 - 2mV_0} \qquad (29)$$

In order Eq. (12) be true ($S \geq 1$), one must take $P \geq \frac{1}{2}$ for any l including $l = 0$.

It follows that the second solution in (29) must be rejected and it is the first regular proof for avoiding this solution (remark that in physical literature there is no unambiguous point of view in this respect. See, e.g. book of R.Newton [14].
and various more modern papers [6,7]. In most papers authors consider only square integrability of wave function and tried to perform a Self-adjoint extension (SAE) procedure on the radial Hamiltonian, eq. (16) [6,7]. As we saw, square integrability is not always sufficient for this purpose. On the other hand, if we impose above boundary condition with $S \geq 1$, then content ourselves with the first solution only $(d_2 = 0)$, the radial Hamiltonian becomes a Self-adjoint and SAE procedure is not necessary, because orthogonality is guaranteed. As regards of the regular solution (the first term in (29)), the condition $P \geq \frac{1}{2}$ is achieved only for

$$l(l+1) > 2mV_0\,. \qquad (30)$$

Remark: for $l = 0$ only repulsive potential is permissible $(V_0 < 0)$.

We do not consider here more complicated singular potentials, but the general tendency is obvious. It follows that Eq. (12) may be applied only for regular potentials. As regards of transitive or more singular potentials – only in cases, when this additional constraint $u(0) = 0$ is fulfilled!

Conclusion: The radial Schrodinger equation in the usual form (12) is valid or have status (Is equivalent (15) to full Schrodinger equation!) only if its solution obeys the (17) boundary behavior $\underset{r\to 0}{u(r)} \approx r^s, \quad with \quad s \geq 1$ at least.

It follows that this (12) equation may be applied only for regular potentials,for singular repulsive potentials and for singular attractive potentials only in cases

$$l(l+1) > 2mV_0$$

when is fulfilled!

In [4,5] articles we noticed, that
problem with delta function arises only in the course of elimination of the first derivative in the equation

$$\frac{d^2R}{dr^2}+\frac{2}{r}\frac{dR}{dr}+2m[E-V(r)]R-\frac{l(l+1)}{r^2}R=0 \qquad (31)$$

We can now show, that if we work with $R(r)$ functions no physical difficulties arises! Indeed (31) equation for (28) singular potentials has such a behaviour at the origin

$$\underset{r\to 0}{R} \approx Ar^{-\frac{1}{2}+P}+Br^{-\frac{1}{2}-P} \qquad (32)$$

In [4] article we show, that requirement of finitness of

$dW=|R(r)|^2r^2dr\sin\theta d\theta d\varphi$ **probability and the time independence of the norm (conservation of particles number!) gives $n>-1$, where**

$$\underset{r\to 0}{R(r)} \approx r^n \qquad (33)$$

or $R(r)$ does not diverge more quickly than $1/r^n$, with $n<1$

So for $P \geq \frac{1}{2}$ in (32) we keep only first term and for $0 \leq P < 1/2$ interval or when is fulfilled condition

$$l(l+1)<2mV_0 \qquad (35)$$

we keep also second term in (32)!

5. Summary

a) We obtain the delta-function like singularity in course of reduction of the Laplace operator in spherical coordinates, which was unnoted till now. Using this observation we proved that this term remains in the radial Schrodinger equation and for its elimination it is necessary to impose curtain restriction on the radial wave function $\underset{r\to 0}{u(r)} \approx r^s, \quad with \quad s \geq 1$ at least.

b) We exposed up the status of (31) radial Schrodinger equation. In particular, we show that (31) radial equation for $R(r)$ function is equivalent (15) to full Schrodinger equation only if its solution $R(r)$ does not diverge at the origin more quickly than $1/r^n$, with $n<1$

c) We also show that, the radial Schrodinger equation in the usual form (12) is valid or have status (Is equivalent (15) to full Schrodinger equation!) only if its solution obeys the (17) boundary behavior $\underset{r\to 0}{u(r)} \approx r^s, \qquad with \quad s \geq 1$ **at least.**

It follows that this (12) equation may be applied only for regular potentials, for singular repulsive potentials and for singular attractive potentials only in cases

$$l(l+1) > 2mV_0$$

when is fulfilled!

For $0 \leq P < 1/2$ **interval or when is fulfilled following condition**

$$l(l+1) < 2mV_0$$

for singular attractive potentials we can't use the well known substitution

$$R(r) = \frac{u(r)}{r}, \qquad \textbf{(36)}$$

d) Lastly, we note that the same holds for radial reduction of the Klein-Gordon equation, because in three dimensions it has the following form

$$\left(-\Delta + m^2\right)\psi(\vec{r}) = [E - V(r)]^2 \psi(\vec{r}) \qquad \textbf{(37)}$$

and the reduction of variables in spherical coordinates will proceed to absolutely same direction as in Schrodinger equation. Here now instead of (28) condition we have

$$\lim_{r\to 0} r\ V(r) = -V_0 = const; \qquad \textbf{(38)}$$

or Coulomb potential is singular potential for the Klein-Gordon equation.

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