Singular Behaviour of the Laplace Operator in Polar coordinates

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1. Introduction

The aim of this talk is to discuss the singular behaviour of the Laplacian in spherical coordinates. Laplacian is encountered almost in all fields of Theoretical physics as well as in mathematical physics. In this article our attention is paid mostly to the Schrodinger equation, which in the Cartesian coordinates has a form (in units $\hbar = c = 1$)

$$\left[-\frac{1}{2m}\Delta + V(r)\right]\psi(\boldsymbol{r}) = E\psi(\boldsymbol{r}); \tag{1}$$

where

$$\Delta \equiv \nabla \cdot \nabla = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$$

(2)

is a Laplacian.

In spherical coordinates the variables are separated and the total wave function is represented as

$$\psi(\boldsymbol{r}) = R(r)Y_l^m(\theta,\varphi) = \frac{u(r)}{r}Y_l^m(\theta,\varphi)$$

(3)

The Laplacian is also rewritten in these coordinates and after the substitution Eq. (3) into the Eq. (1) we derive the radial equations

$$-\frac{1}{2m}\left[\frac{d^2}{dr^2}+\frac{2}{r}\frac{d}{dr}\right]R(r)+\frac{l(l+1)}{2mr^2}R(r)+V(r)R(r)=ER(r)$$

(4)

or

$$\left[-\frac{1}{2m}\frac{d^2}{dr^2}+\frac{l(l+1)}{2mr^2}+V(r)\right]u(r)=Eu(r)$$

(5)

All of this is well known from the classical textbooks on quantum mechanics. We display them here for further practical purposes.

As is well known, in textbooks two methods are used for the transition from Eq. (4) to Eq. (5).

1. the first is a direct substitution in Eq. (4) of the relation

$$R(r)=\frac{u(r)}{r}$$

2. the second method represents the operator in parenthesis of Eq.(4) in the following form

$$\left[\frac{d^2}{dr^2}+\frac{2}{r}\frac{d}{dr}\right]\Rightarrow\frac{1}{r}\frac{d^2}{dr^2}(r.)$$

By unknown reason in both cases the mistake was made.

My talk is devoted for clearing up this point of view.

It will be shown below that the status of the Eq.(5) is problematic.

From both mathematical and physical points of view it is very important that the solutions of radial equations be compatible with the full Schrodinger equation (1).This is verbaly mentioned in books , not only earlier but also in the modern ones [3]. For example,in S.Weinberg"s book "Lectures in Quantum Mechanics"

Earlier **P.Dirac [1] wrote: "Our equations ... strictly speaking, are not correct, but the error is restricted by only one point** $r = 0$.*I t is necessary perform a special investigation of solutions of wave equations, that are derived by using the polar coordinates, to be convince are they valid in the point* $r = 0$ (p.161)"

We are sure that mathematicians knew this problem for a long time, but it was not discussed in physical literature.

The first articles on this subject are:

1. **On the Boundary conditions for the Radial Schrodinger Equation.**
Anzor A. Khelashvili, Teimuraz P. Nadareishvili, (Tbilisi State U. & Georgian U. of Patriarchy) . Jan 2010. 4pp.
e-Print: **arXiv:1001.3285** [math-ph]

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Abstract and Postscript and PDF from arXiv.org (mirrors: au br cn de es fr il in it jp kr ru tw uk za aps lanl)

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2. **Unexpected Delta-Function Term in the Radial Schrodinger Equation.**

Anzor A. Khelashvili, Teimuraz P. Nadareishvili, . Feb 2010. 5pp. e-Print:

arXiv:1002.1278 [math-ph]

LaTeX(US) | LaTeX(EU) | Harvmac | BibTeX

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2. **On the Boundary conditions for the Radial Schrodinger Equation.**
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3. **What is the boundary condition for the reduced radial wave function in the Schrodinger equation.**
Anzor A. Khelashvili, Teimuraz P. Nadareishvili, (Tbilisi State U. & Georgian U. of Patriarchy) .

Am. J. Physics., 79,668 (2011); ArXiv: 1009.2694v2

4. **Singular behaviour of the Laplace operator in spherical coordinates;**

Anzor A. Khelashvili, Teimuraz P. Nadareishvili, (Tbilisi State U. & Georgian U. of Patriarchy) . Bulletin of the Georgian Nat.Acad. of Science (*Moambe*), **6,**68(2012), ArXiv: 1102, 1185v2.

5. **Laplacian in polar coordinates, regular singular function algebra, snd theory of distributions**
   Y.C. Cantelaube and A.L.Khelif. (sounds as ...)
   Journ. of Math.Physics, 51, 053518 May (2010))
6. **Solutions of the Schrodinger equation, boundary condition at the origin, and the Theory of distributions.**
   Y.C. Cantelaube; ArXiv:1203.0551v1; [math-ph] , March 5, 2012.

In the last two papers the problem is formulated as the difference between spaces R(n) and R(n)/{0} from the positions of generalised functions or distribution theory.

You see that the two groups publish papers almost parallel of each others.

The last authors mentioned that :

" In no handbook of quantum mechanics (no article in our knowledge) the radial equation is derived from SE by taking the Laplacians of Ψ and $R(r)$ in the sence of distributions as it is required, but in the sense of function"

Now there appears several citations on our papers.

Because all information is concentrated in the Laplace operator, we begin by consideration the Laplace equation in the vacuum (elecrostatic equation).

1. The Laplace equation

Let us consider the Laplace equation in vacuum

$$\nabla^2 \varphi(\vec{r}) = 0$$

(8)

which in Cartesian coordinates has the form

$$\nabla^2 \varphi(\boldsymbol{r}) = \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) \varphi(x, y, z) = 0$$

(9)

Last equation may be solved simply by separation of variables. The solution has the form [9]

$$\varphi(x, y, z) = e^{\pm i\alpha x} e^{\pm i\beta y} e^{\pm\sqrt{\alpha^2 + \beta^2} z}$$

(10)

Clearly the solution is regular everywhere and at the origin is

$$\varphi(0) = const$$

(11)

There are another forms of solution of Eq.(9) depending on alternate ways of separation, but all of them gives the constant values at the origin.

Now, let us find the spherically symmetric solution. The corresponding equation is written as [Feynmann, 10]

$$\left(\frac{d^2}{dr^2}+\frac{2}{r}\frac{d}{dr}\right)\varphi(r)=0$$

(12)

Certainly, it was possible to pass to spherical coordinates in Eq. (9) and take zero angular momentum $l=0$ **. We arrive again to the Eq. (12).**

The operator in parenthesis of Eq. (12) often is rewritten as ([R.Feynmann], Ch.20, [11] etc.)

$$\frac{1}{r}\frac{d^2}{dr^2}(r\,\cdot)$$

(13)

Correspondingly the Eq. (12) takes the form

$$\frac{1}{r}\frac{d^2}{dr^2}(r\varphi)=0$$

(13a)

the solution of which is

$$u(r)\equiv r\varphi=ar+b$$

(14)

But, determining from here the function

$$\varphi=a+\frac{b}{r}$$

(15)

does not obey to Eq. (12), because

$$\left(\frac{d^2}{dr^2}+\frac{2}{r}\frac{d}{dr}\right)\left(\frac{1}{r}\right)=-4\pi\delta^{(3)}(\boldsymbol{r})$$

(16)

i.e. the function (15) is the solution everywhere except the origin of coordinates. It does not satisfy to the boundary value (11) as well.

What happens? ***It seems that we made an illegal action somewhere (see, R. Feynmann).***

It is possible to consider this problem by another way also, namely, substitute the expression

$$\varphi(r)=\frac{u(r)}{r}$$

(17)

into the Eq.(12) in order to remove the first derivative term. Then we obtain

$$\frac{1}{r}\left(\frac{d^2}{dr^2}+\frac{2}{r}\frac{d}{dr}\right)u(r)+u(r)\left(\frac{d^2}{dr^2}+\frac{2}{r}\frac{d}{dr}\right)\left(\frac{1}{r}\right)+2\frac{du}{dr}\frac{d}{dr}\left(\frac{1}{r}\right)=0$$

(18)

The last term canceles the first derivative in the first parenthesis and there remains

$$\frac{1}{r}\frac{d^2u}{dr^2}+u\left(\frac{d^2}{dr^2}+\frac{2}{r}\frac{d}{dr}\right)\left(\frac{1}{r}\right)=0$$

(19)

the second term is zero by naive calculation. But really, according to Eq. (16), it follows

$$\frac{1}{r}\frac{d^2u}{dr^2}-4\pi\delta^{(3)}(\mathbf{r})u(r)=0$$

(20)

The appearance of the delta function is unexpected. Comparing this one with Eq. (13) we conclude that the representation of the Laplace operator in the form (13) is not valid *everywhere*. The correct form is

$$\frac{d^2}{dr^2}+\frac{2}{r}\frac{d}{dr}=\frac{1}{r}\frac{d^2}{dr^2}(r\,\cdot)-4\pi\delta^{(3)}(\boldsymbol{r})r\,\cdot$$

The last term is not zero!

This expression defines the form of the Laplacian precisely *everywhere* including the origin of coordinates.

By unknown for us reasons this simple fact stayed unnoted till now and in all papers as well as in all books the expession (13) was used. Even in Weinberg's book. As we made clear up above, in this case the obtained solution (15) looks like if there is a point source at the origin. However it is not so – mathematic reason is that in spherical coordinates the point $r=0$ **is absent. The Jacobian of transformation to spherical coordinates has a form**

$J=r^2\sin\theta$ **and is singular at points** $r=0$ **and** $\theta=n\pi \quad (n=0,1,2,...)$

Singularity in angle is eliminated by requirements of continuity and uniquiness, which lead to spherical harmonics $Y_l^m(\theta,\varphi)$. **As regards of the radial variable r there is no such restriction for it. Mathematicians consider**

$r > 0$ strictly. Then all is OK. But in the full 3-dim. equation we need behaviour *everywhere*, including the origin.

Therefore if we want to derive the solution legimitated everywhere, we are forced to include the delta function in consideration. It seems so that,in potential problems, such as e.g. in the Schrodinger equation or another wave equations, where the Laplacian presents, together with the considered potentials we must add the $\delta^{(3)}(\boldsymbol{r})$ potential. It is physically non-sense, of course.

The question is: how to formulate the problem so that to remain all results derived earlier for for the central potentials with the aid of traditional radial equation (5) containing the second derivative only? One of the reasonable way is the following: Because in spherical coordinates $\delta^{(3)}(\vec{r}) = \frac{\delta(r)}{4\pi r^2}$, the Eq. (20) can be reduced to

$$r\frac{d^2u}{dr^2} - \delta(r)u(r) = 0 \tag{22}$$

or

$$r\frac{d^2u}{dr^2} - u(0)\delta(r) = 0 \tag{23}$$

Let us require that the additional term does not present, i.e.

$$u(0) = 0 \tag{24}$$

Moreover the delta function be "overcome" (will be killed) if at least

$$\lim_{r\to 0} u(r) \approx r$$

(25)

Then, owing to the relation $r\delta(r) = 0$ **, the extra term falls out and the standard equation (13) remains. Let us look what the Eq. (24) gives in above considered solution (14). Requiring (24) it follows** $b = 0$ **, i.e.** $u = ar$ **and** $\varphi(r) = a = const$ **. Hence we obtain the correct consisting with the full equation (8) value (11). It is consisting also with the real physical picture.**

Electric potential in vacuum is constant

Appearance of this condition is purely geometrical (not a dynamical) artefact.

Now, what happens in the Schrodinger equation

2. The radial Schrodinger equation

As an example let us consider the radial Schrodinger equation

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

(26)

After the substitution

$$R(r) = \frac{u(r)}{r}$$

(27)

according to abovementioned about the Laplace operator we get

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

(28)

To single out the true singularity let us integrate by dr **in a sphere of small radius** a**. We derive**

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

(29)

From here we determine

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

(30)

Because of smallness of a **substitute here the asymptotic form of wave function at the origin**

$$\underset{r\to 0}{u(r)}\approx r^s \qquad (31)$$

and the potential as

$$\underset{r\to 0}{V(r)}\approx\frac{g}{r^n};n>0 \qquad (32)$$

Then the integration in Eq. (30) may be performed simply and we obtain

$$u(0)=\left[\frac{s(s-1)-l(l+1)}{s}r^{s}+\frac{2mE}{s+2}r^{s+2}-\frac{2mg}{s+2-n}r^{s+2-n}\right]_{0}^{a} \qquad \textbf{(33)}$$

We must remove the extra term from Eq.(23), because otherwise we do not get the usual form of radial equation (5).

If we retain $u(0)$ in Eq. (28) then there are 3 possible values for it:

$u(0)=0$ **;** $u(0)=\mathit{finite}$ **and** $u(0)=\infty$ **. Note that all the enumerated values do not contradict to normalisation condition at the origin**

$\int_0^a u^2 dr < \infty$ ***,*** **but not all of them are permissible.**

The first value is prefarable among them, because finite $u(0)$ will give

$R \approx \frac{const}{r}$ **at the origin**

and in Eq. (26) the delta function reappears again. Therefore this solution will not obey to the full Schrodinger equation. The last value, $u(0)=\infty$ of course is unacceptible also, because to have an infinite number in equation has no sense

There remains only one reasonable value, Eq. (24). Moreover this restriction takes place in spite of the potential is regular or singular. Singularity of the potential effects only on the law of turning $u(r)$ to zero. This follows from the relation (29) as all the exponents here must be positive. We'll have therefore

$$s>0, \quad s+2>0, \quad s+2-n>0$$

moreover $s>1$

It follows from the last inequality that when the index of singularity of potential n increases the index of wave function behaviour must also increase. Moreover we must have $s \geq 1$ in order the wave function at the origin "overcome" the delta function in the term $u(r)\delta(r)$. Interesting enogh that If in addition if we require that this production be a distribution, it become necessary that $u(r)$ be an infinitely smooth function [12,13], i.e. in Eq.(31) we must have $s \geq 1$ and are digital numbers.

Thus the wave function must be sufficiently regular one at the origin.

This conclusion may have many far reaching consequences.

Conclusions

1. **We have found a singularity like the Dirac delta function in process of reduction the Laplace equation in spherical polar coordinates, that was not mentioned earlier. The cornerstone in our consideration is an idea of Dirac that the solution of the radial equation at the same time must be a solution of the full 3-dimensional equation.**
2. **On the basis of this observation we have proved that for removing this extra term from the radial equation it is necessary and sufficient to impose the reduced radial wave function by definite restriction, which has a form of the boundary condition at the origin , eq. (24). Moreover this condition is independent of whether the potential in the Schrodinger equation is regular or singular. The behaviour of singular potential influences only the character of turning to zero of the radial function at the origin.**
3. **As regards of the full radial function $R(r)$, its equation is compatible with the primary (3-dimensional) equation (1) if the restriction**

$$\lim_{r \to 0} rR = 0$$

is satisfied. Therefore, to avoid the misunderstandings, it is preferable to use the equations (26) and (44), for $R(r)$

It was mentioned in *Y.C.Cantelaube et al, arXiv: 1203.0551*

that there is no necessity in putting the boundary condition (24), but instead it is sufficient to require regularity of the solutions of the full radial equation. May be it is a mathematical thinness , we agree. However, it is easy to see from the relation (27) that this requirement is equivalent to our restriction (24).

4. **Let us underline at least that because the Laplacian is encountered in many subjects of physics, our observation can be equally extended to all such problems.**

The same takes place in higher dimensions (more than 3) as well.

Appendicies:

A) Regular potentials

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

Solution at the origin

$$\underset{r\to 0}{u} \sim c_1 r^{l+1} + c_2 r^{-l};\ l = 0,1,2...$$

$$c_2 = 0$$

B) Weakly singular (transition) potential

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

Here $V_0 > 0$ **corresponds to the attraction. Behaviour at the origin**

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

we must have $P \geq \dfrac{1}{2}$

and at the same time

$$1/2 + P = N; \quad N = 1,2,3...$$

It follows that the second solution in Eq. (38) must be discarded in case of attraction.

C) The Klein-Gordon equation

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

Its radial form is

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

Even the Coulomb potential is singular here. Now

$$\lim_{r\to 0} rV(r)=0 \qquad \text{- regular}$$

$$\lim_{r\to 0} rV(r)=-V_0=const \qquad \text{- singular}$$

Now the reduced equation

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

is not applicable even for repulsive case, since the additional contribution for Coulomb potential is quadratic in the coupling constant and is same both for attraction and repulsion.

Therefore this equation may be used for potentials, which are less singular, than the Coulomb one.

Whereas in using of equation for R(r)-function no trubles appear.

D) The Yukawa potential

As a last application of Eq. (21) let us consider the Yukawa potential. According to common viepoint (see, e.g. [Feynman],Ch.28) the Yukawa potential is a spherically symmetric solution of the wave equation

(Helmholtz equation)

$$\nabla^2\phi - \mu^2\phi = 0$$

By "old" consideration it follows that $\phi = K\,\dfrac{e^{-\mu r}}{r}$

But the correct relation gives

$$\nabla^2\,\frac{e^{-\mu r}}{r} = \mu^2\,\frac{e^{-\mu r}}{r} - 4\pi\delta^{(3)}(\boldsymbol{r})e^{-\mu r}$$

Therefore Yukawa potential is the solution of the wave equation with a source term on the RHS:

$$\nabla^2\phi - \mu^2\phi = -4\pi K\delta^{(3)}(\boldsymbol{r})$$

But this "source" is not physical (!)

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

$$\int_0^\infty R_1 H_r R_2 r^2 dr - \int_0^\infty R_2 H_r R_1 r^2 dr =$$

$$= \frac{1}{2} \lim_{r\to 0} \left[u_2(r) u_1'(r) - u_1(r) u_2'(r) \right] = 0$$