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Physics

Delta-Like Singularity in the Radial Laplace Operator and the Status of the Radial Schrödinger Equation

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ABSTRACT. By careful exploration of separation of variables into the Laplacian in spherical coordinates, we obtain the extra delta-like singularity, elimination of which restricts the radial wave function at the origin. This constraint has the form of boundary condition for the radial Schrödinger equation. *© 2012 Bull. Georg. Natl. Acad. Sci.*

Key words: *Laplace operator, radial equation, boundary condition, singular potentials.*

1. Introduction.

It is well known that the Laplace operator appears in many physical as well as of mathematical problems. Especially in quantum mechanics the dynamics of any physical system is described by the three-dimensional Schrödinger equation [1,2]

$$\Delta\psi(\vec{r}) + 2m\left[E - V(r)\right]\psi(\vec{r}) = 0. \qquad (1)$$

The central potential $V(\vec{r}) = V(|\vec{r}|) \equiv V(r)$ is frequently encountered in most interesting physical problems, therefore reduction to the one-dimensional (radial) equation is a widespread procedure.

The traditional way is the application of the substitution $\psi(\vec{r}) = R(r)\mathrm{Y}_l^m(\theta,\varphi)$, where $\mathrm{Y}_l^m(\theta,\varphi)$ is the spherical harmonics and because of the continuity and uniqueness, orbital quantum numbers l are integers, $l = 0,1,2,...,$ whereas $m = -|l|,...,l.$

After this substitution angular variables are separated and we are left with the equation for the full radial function $R(r)$

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

It is a traditional trick in quantum mechanics to avoid the first derivative term from this equation by substitution

$$R(r) = \frac{u(r)}{r} \qquad (3)$$

after which a naïve calculation gives the equation for the new radial wave function $u(r)$ in the form

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

It is this equation that plays an important role in quantum mechanics since its birth. However, as has been clarified in recent years, there is an ambiguity in derivation of boundary condition for $u(r)$ at the origin r=0, especially in the case of singular potentials [3-5].

According to this reason many authors content themselves by consideration only of a square integrability of radial function and do not pay attention to its behavior at the origin. Of course, this is permissible mathematically and the strong theory of linear differential operators allows for such an approach [6-8]. There appears the so-called self-adjoint extended (SAE) physics [9], in the framework of which among physically reasonable solutions one encounters also many curious results, such as bound states in the case of repulsive potential [10] 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 Schrödinger Hamiltonian is not restricted correctly..

Careful investigation, performed below, shows that the validity of radial equation (4) is not correctly established. Indeed, it is physically (and mathematically, of course) warranted that the equation, obtained after separation of variables, must be compatible with the primary equation. It is a necessary condition for the correctness of a separation procedure.

2. Rigorous derivation of radial equation.

In the case of reduction of Laplace operator the transition from Cartesian to spherical coordinates is not unambiguous, because the Jacobian of this transformation [11] $J = r^2 \sin\theta$ is singular at $r = 0$ and $\theta = n\pi\,(n = 0,1,2,...)$. The angular part is fixed by the requirement of continuity and uniqueness. This gives the unique spherical harmonics $Y_l^m(\theta,\varphi)$ mentioned above.

Note that in the reduction of Laplace operator it usually is pointed out that $r > 0$. However, $\vec{r} = 0$ is an ordinary point in the full Schrödinger equation (1), but it is a point of singularity in the reduction of variables. Thus, the knowledge of specific boundary behavior is necessary. We underline that the equation (2) is correct, but the substitution (3) enhances singularity at r=0 and may cause some misunderstandings.

Indeed, let us rewrite the full radial equation (2) after this substitution

$$\frac{1}{r}\left(\frac{d^2}{dr^2}+\frac{2}{r}\frac{d}{dr}\right)u(r)+u(r)\left(\frac{d^2}{dr^2}+\frac{2}{r}\frac{d}{dr}\right)\left(\frac{1}{r}\right)+ +2\frac{du}{dr}\frac{d}{dr}\left(\frac{1}{r}\right)-\left[\frac{l(l+1)}{r^2}-2m\left(E-V(r)\right)\right]\frac{u}{r}=0. \quad (5)$$

We write the equation in this form deliberately, indicating the action of radial part of Laplacian on relevant factors explicitly. It seems that the first derivatives of $u(r)$ are cancelled and we are faced with the following equation

$$\frac{1}{r}\left(\frac{d^2u}{dr^2}\right)+u\left(\frac{d^2}{dr^2}+\frac{2}{r}\frac{d}{dr}\right)\left(\frac{1}{r}\right)- -\frac{l(l+1)}{r^2}\frac{u}{r}+2m\left(E-V(r)\right)\frac{u}{r}=0. \quad (6)$$

Now if we differentiate the second term "naively", we'll derive zero. But it is true only in the case when $r \neq 0$. However, below we show that in general this term is proportional to the 3-dimensional delta function. Indeed, taking into account that

$$\frac{d^2}{dr^2}+\frac{2}{r}\frac{d}{dr}=\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{d}{dr}\right)\equiv\Delta_r \quad (7)$$

is the radial part of the Laplace operator and therefore [12]

$$\Delta_r\left(\frac{1}{r}\right)=\Delta\left(\frac{1}{r}\right)=-4\pi\delta^{(3)}(\vec{r}) \quad (8)$$

we obtain the equation for $u(r)$

$$\frac{1}{r}\left[-\frac{d^2u(r)}{dr^2}+\frac{l(l+1)}{r^2}u(r)\right]+4\pi\delta^{(3)}(\vec{r})u(r)$$

$$-2m\left[E-V(r)\right]\frac{u(r)}{r}=0. \qquad (9)$$

We see that there appears the extra delta-function term. Its presence in the radial equation is physically nonsense and must be eliminated. Note that when $r \neq 0$, this extra term vanishes owing to the property of the delta function and if, in this case, we multiply this equation by r, we'll obtain an ordinary radial equation (4).

However if $r=0$, multiplication by r is not permissible and this extra term remains in Eq. (9). Therefore one has to investigate this term separately and find another ways to abandon it.

The term with 3-dimensional delta-function must be comprehended as being integrated over $d^3r = r^2 dr \sin\theta d\theta d\varphi$. On the other hand [12]

$$\delta^{(3)}(\vec{r}) = \frac{1}{|J|}\delta(r)\delta(\theta)\delta(\varphi), \qquad (10)$$

where $J = r^2 \sin\theta$ is the Jacobian of transformation.

Taking into account all the above mentioned relations, one is convinced that the extra term still survives, but now in the one-dimensional form

$$u(r)\delta^{(3)}(\vec{r})d^3\vec{r} \to u(r)\delta(r)dr. \qquad (11)$$

Its appearance as a point-like source breaks many fundamental principles of physics, which is not desirable. The only reasonable way to remove this term without modifying Laplace operator or including compensating delta function term into the potential $V(r)$, is to impose the requirement

$$u(0)=0 \qquad (12)$$

(note that multiplication of Eq. (9) by r and then elimination of this extra term owing to the property $r\delta(r)=0$ is not a legitimate procedure, because effectively it is equivalent to multiplication by zero).

Therefore we conclude that the radial equation (4) for $u(r)$ is compatible with the full Schrödinger equation (1) if and only if the condition $u(0)=0$ is fulfilled. *The radial equation (4) supplemented by the condition (12) is equivalent to the full Schrödinger equation (1).* It is in accordance with the Dirac requirement [2], that the solutions of the radial equation must be compatible with the full Schrodinger equation. It is remarkable to see that the supplementary condition (12) has a form of boundary condition at the origin.

3. Comments, some applications and conclusions

Some comments are in order here: equation for $R(r) = \frac{u(r)}{r}$ has its usual form (2). Derivation of boundary behavior from this equation is as problematic as for $u(r)$ from Eq. (4). Problem with delta function arises only in the course of elimination of the first derivative. Now, after the condition (12) is established, it follows that the full wave function $R(r)$ is less singular at the origin than r^{-1}. However, this conclusion could be hasty because the transition to Eq. (4) for $R(r)$ is not necessary at all. It is also remarkable to note that the boundary condition (12) is valid whether potential is regular or singular. It is only the consequence of particular transformation of Laplacian. Different potentials can only the determined in the specific way of $u(r)$ tending to zero at the origin and the delta function arises in the reduction of the Laplace operator every time. All of these statements can easily be verified also by explicit integration of Eq. (9) over a small sphere with radius a tending to zero at the end of calculations.

It seems very curious that this fact has hitherto remained unnoticed by physicists in spite of numerous discussions [1, 2].

Apparently mathematicians knew about the singular behavior of Laplace operator for a long time. But their results did not find a relevant presentation in physical literature, while the delta function became popular only after Dirac. Therefore the fact, described above, seems to us as being very curious.

We discuss another important point with regard to radial Laplacian. It is well known from some books on special functions that there is the following operator relation [12]

$$\Delta_r = \frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{d}{dr}\cdot\right) = \frac{1}{r}\frac{d^2}{dr^2}(r\,\cdot). \qquad (13)$$

Here the dot denotes the impact of this expression on some function. The validity of this relation is easily verified by direct calculation. But this equality fails at point $r = 0$. Indeed, let us act by both sides on the full radial function $R(r)$:

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) = \frac{1}{r}\frac{d^2}{dr^2}(rR) = \frac{1}{r}\frac{d^2}{dr^2}u(r). \qquad (14)$$

It is this relation that is used in mathematical literature for special functions [13].

If it is true everywhere, then there does not appear any problem in the derivation of the radial equation. But now we know that after substitution of $R(r) = \dfrac{u(r)}{r}$ on the left-hand side it follows

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{d}{dr}\frac{u}{r}\right) = \frac{1}{r}\frac{d^2u}{dr^2} - 4\pi\delta(\vec{r})u. \qquad (15)$$

Therefore previous operator equality must be modified perhaps as follows

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{d}{dr}\cdot\right) = \frac{1}{r}\frac{d^2}{dr^2}(r\,\cdot) - 4\pi\delta^{(3)}(\vec{r})r\,\cdot. \qquad (16)$$

This relation is correct at every point including the origin. The validity of this relation may be checked by acting on $R(r)$, and then using equality $u = rR$.

The relation $u(0) = 0$ is not only the boundary condition for the radial equation, but it is a relation which must be necessarily fulfilled in order to have the radial equation in its usual form compatible to the full Schrödinger equation. Accidentally it has a boundary condition form. Without this condition the radial equation is not valid.

Now, after this condition has been established, many problems can be considered rigorously by taking it into account. Remarkably, all the results obtained earlier for regular potentials with the boundary condition (12) remain unchanged. In most textbooks on quantum mechanics $r \to 0$ behavior is obtained from Eq. (4) in the case of regular potentials. When an equation like (4) is known, the derivation of boundary behavior from it is an almost trivial procedure. It depends on the behavior of the potential under consideration.

But we have shown that this equation takes place only together with a boundary condition (12). On the other hand, for *singular potentials* this condition will have far-reaching implications. Many authors neglected the boundary condition entirely and were satisfied only by square integrability. But in this treatment some parameters of wave functions go out of allowed regions and a self-adjoint extension procedure can yield unphysical results. Below we consider some simple consequences showing the differences which arise with and without the above mentioned boundary condition:

(i) Regular potentials at the origin:

$$\lim_{r\to 0} r^2 V(r) = 0. \qquad (17)$$

In this case, after substitution at the origin of $u \sim r^s$, it follows from inicial equation that $s(s-1) = l(l+1)$, which gives two solutions $\underset{r\to 0}{u} \sim c_1 r^{l+1} + c_2 r^{-l}$ (see, any textbooks on quantum mechanics). For non-zero l-s the second solution is not square integrable and is usually ignored. But for $l = 0$, many authors discuss how to deal with this solution [14], which is also square integrable near the origin. According to condition (12), this solution must be ignored. This result justifies the assumption made in the book of A.Messiah [15] about the behavior of the s-state wave function at the origin.

(ii) Transitive attractive singular potentials at the origin:

$$\lim_{r\to 0} r^2 V(r) = -V_0 = const; \qquad V_0 > 0. \qquad (18)$$

In this case, the indicial equation takes the form $s(s-1) = l(l+1) - 2mV_0$, which has two solutions: $s = \frac{1}{2} \pm \sqrt{\left(l + \frac{1}{2}\right)^2 - 2mV_0}$. Therefore

$$u \underset{r \to 0}{\sim} c_1 r^{\frac{1}{2}+P} + c_2 r^{\frac{1}{2}-P}; \quad P = \sqrt{\left(l + \frac{1}{2}\right)^2 - 2mV_0}. \quad (19)$$

It seems that both solutions are square integrable at origin as long as $0 \le P < 1$. Exactly this range is studied in most papers (see for example [10]), whereas according to boundary condition (12) we have $0 \le P < \frac{1}{2}$. The difference is essential. Indeed, the radial equation has a form

$$u'' - \frac{P^2 - 1/4}{r^2} u + 2mEu = 0. \quad (20)$$

Depending on whether P exceeds 1/2 or not, the sign in front of the fraction changes and one can derive attraction in the case of repulsive potential and vice versa. Boundary condition (12) avoids this nonphysical region $\frac{1}{2} \le P < 1$.

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

$$\left(-\Delta + m^2\right)\psi(\vec{r}) = \left[E - V(r)\right]^2 \psi(\vec{r}) \quad (21)$$

and the reduction of variables in spherical coordinates will proceed in an absolutely same direction as in Schrödinger equation. Interestingly enough, something like that arises in classical electrodynamics [16] in calculations of electric dipole and magnetic fields, but cancels without any physical consequences. The situation in quantum mechanics differs because the extra delta term necessitates the restriction of the radial wave function.

ფიზიკა

დელტასმაგვარი სინგულარობა რადიალურ ლაპლასის ოპერატორში და შრედინგერის რადიალური განტოლების სტატუსი

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