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Physics

On the Boundary Conditions for the Radial Schrödinger Equation

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ABSTRACT. We show that an equation for the radial wave function is compatible with the full three-dimensional Schrödinger equation if and only if a definite boundary condition is imposed on the radial wave function at the origin.

Key words: *full Schrödinger equation, radial equation, Laplace operator, singular potentials.*

1. Introduction.

It is well known that the radial Schrödinger equation

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

plays a central role in quantum mechanics due to frequent encounter with spherically symmetric potentials. As is well known this equation is obtained from the full 3-dimensional Schrödinger equation

$$\Delta\psi(\vec{\mathbf{r}})+2m\left[E-V(r)\right]\psi(\vec{\mathbf{r}})=0\,, \quad (2)$$

after the separation of variables in the spherical coordinates [1, 2].

Recently considerable attention has been devoted to the problems of self-adjoint extension (SAE) for the inverse squared r^{-2} behaved potentials in the radial Schrödinger equation [3]. These problems are interesting not only from the academic standpoint, but also due to the large number of physically significant quantum-mechanical problems that manifest such behavior.

The Hamiltonians with the inverse squared like potentials appear in many systems and they have sufficiently rich physical and mathematical structures. Beginning with the 1960s, singular potentials were the subject of intensive studies in connection with the non-renormalizable field theoretic models. Exhaustive reviews dedicated to singular potentials for that period can be found in [4-6].

It turned out that there are no rigorous ways of deriving the definite boundary condition for the radial wave function $u(r)$ from the radial equation itself at the origin $r=0$ in the case of the singular potentials.

Many authors content themselves with consideration only of the square integrability of the radial wave function and do not pay attention to its behavior at the origin. Of course this is permissible mathematically and the strong theory of the linear differential operators allows for such approach [7-9]. There appears the so-called SAE physics [3], 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 of a functional domain for the radial Schrödinger Hamiltonian is not restricted correctly [11].

Below we show that, due to the singular character of the transformation which leads to Eq. (1) from Eq. (2), there appears the extra delta function term, which plays a role of point-like source, interacting to the wave function. Surprisingly enough, this term has not been noted earlier. From the requirement of its absence definite constraint follows on the radial wave function at the origin. It has the form of a boundary condition but indeed has more importance than a boundary condition. This fact can exert considerable influence on the further considerations of the radial equation.

2. Rigorous derivation of radial equation.

Let us mention that the transition from Cartesian to spherical coordinates is not unambiguous, because the Jacobian of this transformation $J = r^2 \sin\theta$ 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. It gives the unique spherical harmonics $Y_l^m(\theta,\varphi)$.

We also note that though $\vec{r} = 0$ is an ordinary point in the full Schrödinger equation, it is a point of singularity in the radial equation and thus knowledge of the specific boundary behavior is required.

We have to bear in mind that the Eq.(1) is not independent but is derived from the full 3-dimensional Schrödinger equation (2) and as is underlined in many classical books on quantum mechanics, the final radial equation must be compatible with the primary full Schrödinger equation. Unfortunately, in our opinion, this view has not been extended to any concrete results [2, 12]. Though several discussions of mostly "beat about the bush" nature exist in the literature (see, e.g. the book of R. Newton [13]), the conclusions from these studies are largely conservative and cautious. It seems that without deeper exploration of the idea of compatibility, some significant point will be missed.

Armed with this idea, let us now look at the derivation of the radial wave equation in more detail. Remembering that, after substitution

$$\psi(\vec{r}) = R(r)Y_l^m(\theta,\varphi) \tag{3}$$

into the 3-dimensional Equation (2), it follows the usual equation for the full radial function $R(r)$:

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

A traditional trick of avoiding the first derivative term from this equation consists in the substitution

$$R(r) = \frac{u(r)}{r}. \tag{5}$$

This substitution enhances the singularity at $r = 0$, therefore we must be careful to perform it. Let us rewrite the equation (4) after this substitution

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

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

We write the equation in this form deliberately, showing the action of the radial part of the Laplacian on relevant factors explicitly. The first derivatives of $u(r)$ cancel and we are left with

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

$$-\frac{l(l+1)}{r^2}\frac{u}{r} + 2m\left(E - V(r)\right)\frac{u}{r} = 0. \tag{7}$$

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

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

is the radial part of the Laplace operator and [14]

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

we obtain the equation for $u(r)$

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

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

We see that there appears an extra 3-dimensional delta-function term. Its presence in the radial equation has no physical meaning and thus it must be eliminated. Note that when $r \neq 0$, this extra term vanishes due to the property of the delta function and also if $r \neq 0$ and we multiply this equation by r, we obtain the ordinary radial equation (1). 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 a way to discard 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 [14]

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

where $J = r^2 \sin\theta$ is the Jacobian, as was mentioned in the Introduction.

Taking into account all the above relations, one is convinced that the extra term effectively becomes

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

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

$$u(0) = 0 \tag{12}$$

(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 it is equivalent to multiplication of this term by zero).

Therefore we conclude that the radial equation (1) for $u(r)$ is compatible with the full Schrödinger equation (2) if and only if the condition $u(0) = 0$ is satisfied.

The radial equation (1) supplemented by the condition (12) is equivalent to the full Schrödinger equation (2). We see that the constraint equation has the form of a boundary condition.

3. Conclusions and remarks

Some comments are in order here: the equation for the $R(r) = \frac{u(r)}{r}$ has its usual form (4). Derivation of the boundary behavior from this equation is as problematic as for $u(r)$ from Eq. (1). The problem with the delta function arises only in the process 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. (1) for $R(r)$ is not necessary. It is also remarkable to note that the condition (12) is valid whether the potential is regular or singular. It is only the consequence of particular transformation of the Laplacian. Different potentials can only determine the specific way of $u(r)$ tending to the 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 the radius a tending it to the zero at the end of calculations.

It seems very curious that the appearance of delta functions while reducing the Schrödinger equation was unnoticed up till now in spite of numerous discussions [2,5,6,12,13]. Now, that this (boundary) condition has been established, many problems can be solved by taking it into account. Remarkably, all the results obtained earlier for the regular potentials with the boundary condition (12) remain unchanged. In most textbooks on quantum mechanics $r \to 0$ behavior is obtained from Eq. (1) in the case of regular potentials. But we have shown that this equation takes place only together with the boundary condition (12). On the other hand, for the *singular potentials* this condition will have far-reaching implications. Many authors neglected a boundary condition entirely and were satisfied only with the square integrability [3, 10]. But this treatment, after leakage into the forbidden regions and through a self-adjoint extension procedure, sometimes yields curious unphysical results. Below we consider some simple examples, showing the differences that arise with and without the above-mentioned boundary condition:

(i) Regular potentials

$$\lim_{r\to 0} r^2 V(r) = 0. \tag{13}$$

In this case, after substitution at the origin $u \sim r^a$, it follows from the characteristic equation that $a(a-1) = l(l+1)$, which gives two solutions $u_{r\to 0} \sim c_1 r^{l+1} + c_2 r^{-l}$ (see, any textbook on quantum mechanics). For non-zero l-s the second solution is not square integrable and usually is ignored. But for $l = 0$, many authors discuss (see, e.g. page 352 in [12]) how to deal with this solution, which is square integrable near the origin. According to our result, this solution must be ignored. Moreover, $u_{r\to 0} \sim const$ solution is totally forbidden because there appears the delta-function after its substitution into the full Schrödinger equation. Therefore, we must require $u(0)=0$ for *any l*, which automatically takes place for our constraint.

(ii) Transitive singular potentials

$$\lim_{r\to 0} r^2 V(r) = -V_0 = const. \tag{14}$$

$V_0 > 0$ corresponds to the attraction, while $V_0 < 0$ - to repulsion.

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

$$\underset{r\to 0}{u} \sim c_1 r^{\frac{1}{2}+P} + c_2 r^{\frac{1}{2}-P} \quad ; \quad P = \sqrt{\left(l+\frac{1}{2}\right)^2 - 2mV_0}. \tag{15}$$

It seems that both solutions are square integrable at the origin as long as $0 \le P < 1$. Exactly this range is studied in most papers [3,10].whereas according to our boundary condition (12) we have the following restriction $0 \le P < \frac{1}{2}$. The difference is essential. Indeed, the radial equation takes the form

$$u'' - \frac{P^2 - 1/4}{r^2} u = 2mEu. \tag{16}$$

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. The boundary condition (12) avoids this unphysical region $\frac{1}{2} \le P < 1$.

Notice that the boundary condition at the origin was a subject of fairly many textbooks and scientific articles [15-20]. The authors come to the condition $u(0)=0$ in various ways starting from the radial equation (1). But their considerations are mainly restricted to the case of the regular potentials. As regards singular potentials, there is no common view and people considered the Dirichlet, which coincides with (12), or the Neumann boundary conditions, as well as their generalization – the Robin boundary condition [20]. We underline once again that the derived constraint (12) is valid both for regular as well singular potentials. Note that ignorance of this fact is continued in the recently appearing papers as well [see, e.g. [21]), where only the square integrability is considered.

Moreover, our result above tells that the radial equation by itself is valid only in the case $u(0)=0$. Hence consideration of the boundary behaviors based on the radial equation is improper. It is evident that the deeper mathematical study of the radial Hamiltonian is permissible, but without the constraint (12) these investigations would have only mathematical importance and they have nothing in common with physics, except the case $u(0)=0$.

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

$$\left(-\Delta + m^2\right)\psi(\vec{r}) = \left[E - V(r)\right]^2 \psi(\vec{r}) \tag{17}$$

and the reduction of variables in spherical coordinates will proceed in absolutely the same direction as in the Schrödinger equation.

ფიზიკა

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REFERENCES:

1. *L. Schiff* (1968), Quantum Mechanics. Third Edition, Mc. Graw-Hill Book Company: New York-Toronto-London.
2. *P. Dirac* (1958),The Principles of Quantum Mechanics. Fourth Edition, Univ. Press: Oxford.
3. *P. Giri* (2008), Phys.Lett., **A372**: 2967.
4. *K. Case* (1950), Phys.Rev., **80**: 797.
5. *W. Frank* (1971), Rev.Mod.Phys., **43**: 36.
6. *A. Filippov* (1979), Sov. Journ. Fiz. Elem.Chast.Atom.Yadra, **10**: 501 (In Russian).
7. *N. Akhiezer, I. Glazman* (1993), Theory of Linear Operators in the Hilbert Space. Dover Publications, Inc.: N.Y.
8. *T. Kato* (1995), Perturbation Theory for Linear Operators. Second Edition. Springer-Verlag:Berlin and Heidelberg.
9. *T. Kato* (1951), Trans.Am.Math.Soc., **70:** 195.
10. *H. Falomir et al*. (2004), J.Math.Phys., **45**: 4560.
11. *T. Nadareishvili, A. Khelashvili* (2009), http://_arXiv.org/_abs/0903.0234v4[math-ph].
12. *A. Messiah* (1999), Quantum mechanics. Two Volumes Bound as One. Dover Publications.
13. *R. Newton* (1982), Scattering Theory of Waves and Particles. Second Edition, Springer-Verlag: New York, Heidelberg and Berlin, p.391.
14. *J. Jackson* (1999), Classical Electrodynamics.Third Edition. New York-London, p.120.
15. *A. Nikiforov, V. Uvarov* (1988), Special Functions of Mathematical Physics: a Unified Introduction with Applications. Boston: Birkhauser.
16. *M. Reed, B. Simon* (1978), Methods of Modern Mathematical Physics.Vol. 4.Academic Press: New York.
17. *E. Coddington, N. Levinson* (1955), Theory of Ordinary Differential Equations. Mc. Graw-Hill Book Company:New York-Toronto-London.
18. *T. Jordan* (1976), Am.J.Phys., **44:** 567.
19. *B. Basu-Mallick* (2008), Eur.Phys.J.**C** **58:** 159.
20. *B. Belchev, M. Walton* (2010), J. Phys. A: Math. Theor., **43**: 085301.
21. *D. Sinha, P. Giri* (2010), http://_arXiv.org/_abs 1010.4418 [hep-th].

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