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On the Status of the Radial Schrodinger Equation

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3- dim. Schrodinger Equation

$$\left[-\frac{1}{2m}\Delta+V\left(\boldsymbol{r}\right)\right]\Psi\left(\boldsymbol{r}\right)=0$$

Spherical symmetry $$V\left(\boldsymbol{r}\right)=V\left(\left|\boldsymbol{r}\right|\right)\equiv V\left(r\right)$$

Transition to the spherical coordinates

$$x=r\sin\theta\cos\varphi \qquad 0\le\theta<\pi$$
$$y=r\sin\theta\sin\varphi \qquad 0\le\varphi<2\pi$$
$$z=r\cos\theta \qquad 0<r<\infty$$

Jacobian of Transformation

$$J=r^2\sin\theta$$

has zeros at $r = 0$ and $\theta = n\pi$. Therefore is singular at these points.

Singularitiy in angular variables is arranged by requiring of continuity and unambiguity at critical points. As a result there appears so-called Spherical Harmonics,

$$Y_l^m(\theta, \varphi); \qquad l = 0, 1, \ldots; \qquad -l \le m \le l$$

But what about r ? After the substitution

$\Psi(\boldsymbol{r}) = R(r) Y_l^m(\theta, \varphi)$ into 3D equation, variables are separated and we obtain the Radial equation or equation for <u>full Radial function</u>

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

It is a common practice to eliminate the first derivative term from this equation by following substitution

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

Direct calculation gives the equation for radial wave function $u(r)$

(Reduced radial wave function)

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

All of these is in any textbooks on quantum mechanics.

But let make this last substitution more <u>carefully</u>

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

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

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

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

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

$$\Delta_r\left(\frac{1}{r}\right)$$

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

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Instead of traditional radial equation we obtain equation with extra term, contended 3D - Delta

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

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

$$d^3r = r^2 dr \sin\theta d\theta d\varphi$$

"Effectively"

$$u(r)\delta^{(3)}(\vec{r}) \to u(r)\delta(r)$$

It seems, that

$$u(0) = 0$$

The same happens in the Klein-Gordon Equation

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

Conclusion of Pedagogical part: **In equation for the reduced radial wave function $u(r)$ there appears the extra Delta function term, elimination of which requires restricting a wave function at the origin beforehand. This restriction has a form of vanishing boundary condition**

$$u(0) = 0$$

no matter the potential is regular or singular (!!!)

_It is in
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_A.Khelashvili, T.Nadareishvili, **Am. J. Phys. 79 (6),668 (2011)**

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Another point of view:

Let us denote the radial part of the Laplace operator in spherical coordinates as

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

This form often is written in two alternative compact expressions

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

(2)
and/or

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

(3)
It is easy to check by direct inspection that these two operator expressions are equal to each other's and that of (1):

$$\Delta_1 = \Delta_2 = \Delta_r$$

(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. Now 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 the full radial function $R(r)$ gives

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

(5a)

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

(5b)

Usually a new function, called radial wave function, is used to define

$$u = rR$$

(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.

We already have shown that this fact is correct only in special circumstances, depending on the boundary behavior of the radial wave function.

Appearance of singularity

Let us see what happens if this 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

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

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

(7)

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

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

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 ***modified*** when the origin is included, probably as follows.We propose the followind form[*)]

$$\Delta_1=\Delta_r=\Delta_2-4\pi\delta^{(3)}\left(\boldsymbol{r}\right)$$

(8)

[*)] ***One comment is needed here: the form (8) is correct when we apply both sides on*** $u\left(r\right)$***, but in case of R(r) it is necessary to change as*** $\delta^{(3)}\left(\boldsymbol{r}\right)\to r\delta^{(3)}\left(\boldsymbol{r}\right)$.

2. Some Consequences

Last few decades people considered many times the following Hamiltonian

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

,

which is directly connected to the usual radial equation and they are interested whether this Hamiltonian is self-adjoint.

The condition of self-adjointness for this Hamiltonian means the fulfillment of the following condition

$$\lim_{r\to 0}\left\{u_2(r)\frac{du_1}{dr} - u_1(r)\frac{du_2}{dr}\right\} = 0$$

Where $u_{1,2}(r)$ are two linearly-independent solutions of radial equation.

You see that this requirement is closely related to the boundary behavior of $u(r)$.

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

$$\int_0^\infty |u(r)|^2 dr < \infty$$

Of course, this is permissible mathematically and the strong theory of linear differential operators allows for such an approach. There appears so-called Self-Adjoint Extended (SAE) physics, in the framework of which among physically reasonable solutions one encounters also many curious results, such as bound states in case of repulsive potential 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 is not restricted correctly. As we have seen above, the mentioned expression is a physical Hamiltonian and usual radial equation is correct only if $u(0) = 0$.

To elucidate more clearly the points discussed above, let us investigate the true equation near the origin carefully.

We know 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 ,

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

we must require that $s \geq 1$.

According to previous consideration it is clear:

- We must recognize that the extra delta term is present in the radial equation and try to go further:
- 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 in case of general behaved potential

- $$\underset{r\to 0}{V(r)} \approx \frac{g}{r^n}, \quad n \geq 1$$

- Simple way consists in using the well- known representation for 3-dimensional delta-function in spherical coordinates: There is known two formulae

$$\delta^{(3)}(\vec{r}) = \frac{1}{2\pi r^2}\delta(r)$$

or/and

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

which depends on definition of the sign function.

Below we use the second definition (only for simplicity)

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

Let us integrate this equation inside of a small sphere

$$r^2dr$$

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

and obtain

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

Because of smallness of radius a, we can substitute here asymptotic form of the wave function at the origin in the form

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

and simultaneously, choose the potential at the origin in the abovementioned form.
Then, integration is easily performed and it follows:

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

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

$$u(0)=0; \qquad u(0)-Finite \qquad u(0)=\infty$$

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 reappears 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

$$u(0) = 0$$

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, 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

$$s + 2 - n > 0 \; ; \; , \quad s \geq 1$$

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.

2. Some applications

What does this result mean?

Let now discuss various potentials:

(1) Regular potentials:

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

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

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

It follows that we must retain only the first one even in case of $l = 0$, nevertheless this term does not destroy normalization of wave function near the origin. Simply it is not a solution of full Schrodinger equation

We can conclude here that in case of regular potentials usual equation 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

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

Here $V_0 > 0$ corresponds to the attraction, while $V_0 < 0$ - to repulsion. Now Eq. (10) gives the following behavior at origin

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

In order usual equation be true ($s \geq 1$), one must take $p \geq 1/2$ for any l including $l=0$.
It follows that the second solution 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 and various more modern papers). 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. 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 above, the condition $p \geq 1/2$ is achieved only for $l(l+1) > 2mV_0$. Remark that 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 usual equation may be applied only for regular potentials. As regards of transitive or more singular potentials – only in cases, when this additional constraint is fulfilled.

Thanks for your kind attention.

$$r^2 V(r) \underset{r \to 0}{\longrightarrow} 0$$

$$u_{r\to 0} \sim c_1 r^{l+1} + c_2 r^{-l}$$

$$c_2 = 0$$

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

$$u_{r\to 0} \sim c_1 r^{\frac{1}{2}+P} + c_2 r^{\frac{1}{2}-P} \; ;$$

$$P = \sqrt{\left(l+\frac{1}{2}\right)^2 - 2mV_0}$$

$$P \ge 1/2 \qquad\qquad c_2 = 0$$

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

$$\lim_{r \to 0} \left\{ u_2(r) \frac{du_1}{dr} - u_1(r) \frac{du_2}{dr} \right\} = 0$$